

10509228

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PASSWORD:

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COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.28	5.49

=> file reg

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.72	5.93

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DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> set postings on  
SET COMMAND COMPLETED

=> s heterocyclic and aldehyde  
2 HETEROCYCLIC  
296422 ALDEHYDE  
24 ALDEHYDES  
296422 ALDEHYDE  
(ALDEHYDE OR ALDEHYDES)  
L4 0 HETEROCYCLIC AND ALDEHYDE

Updated Search

10509228

=> s aldehyde?  
L5 296422 ALDEHYDE?

=> s heterocyclic  
L6 2 HETEROCYCLIC

=> s l6 and l5  
L7 0 L6 AND L5

=> s hydroxymethyl  
L8 275636 HYDROXYMETHYL

=> file hcaplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	24.68	30.61

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006  
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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16  
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

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FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

=> s l5/prep  
751488 L5  
3539700 PREP/RL  
L9 144752 L5/PREP  
(L5 (L) PREP/RL)

=>

=> s l8/rct  
458850 L8  
2897022 RCT/RL  
L10 100866 L8/RCT  
(L8 (L) RCT/RL)

=> s l10 (1) l9  
L11 982 L10 (L) L9

=> file hcaplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	15.18	45.79

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006  
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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16  
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s hypohalogenous? () salt?  
53 HYPOHALOGENOUS?  
1175891 SALT?  
L12 1 HYPOHALOGENOUS? (W) SALT?

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006  
L1 STRUCTURE UPLOADED

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L2               STRUCTURE UPLOADED  
L3               6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON

L4               0 S HETEROCYCLIC AND ALDEHYDE  
L5               296422 S ALDEHYDE?  
L6               2 S HETEROCYCLIC  
L7               0 S L6 AND L5  
L8               275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9               144752 S L5/PREP  
L10              100866 S L8/RCT  
L11              982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12              1 S HYPOHALOGENOUS? () SALT?

=> s l12 l11  
MISSING OPERATOR L12 L11  
The search profile that was entered contains terms or  
nested terms that are not separated by a logical operator.

=> s l12 () l11  
PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH  
FIELD CODE - 'AND' OPERATOR ASSUMED 'L12 (W) L11'  
L13              0 L12 (W) L11

=> s l12 and l11  
L14              0 L12 AND L11

=> s halogen?  
L15              166106 HALOGEN?

=> s l15 () l11  
PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH  
FIELD CODE - 'AND' OPERATOR ASSUMED 'L15 (W) L11'  
L16              28 L15 (W) L11

=> s l12 (l) l11  
L17              0 L12 (L) L11

=> s l12 and l11  
L18              0 L12 AND L11

=> s l15 and l11  
L19              28 L15 AND L11

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.59	53.38

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006  
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DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> set postings on  
SET COMMAND COMPLETED

=> s tetramethyl and piperidine  
383162 TETRAMETHYL  
2 TETRAMETHYLS  
383162 TETRAMETHYL  
(TETRAMETHYL OR TETRAMETHYLS)  
394986 PIPERIDINE  
L20 6024 TETRAMETHYL AND PIPERIDINE

=> s l20 and oxyl  
7516 OXYL  
L21 92 L20 AND OXYL

=> s "2,2,6,6-tetramethyl" and piperidine and "1-oxyl"  
32058 "2,2,6,6"  
383162 "TETRAMETHYL"  
2 "TETRAMETHYLS"  
383162 "TETRAMETHYL"  
( "TETRAMETHYL" OR "TETRAMETHYLS" )  
30406 "2,2,6,6-TETRAMETHYL"  
( "2,2,6,6" (W) "TETRAMETHYL" )  
394986 PIPERIDINE  
19346742 "1"  
7516 "OXYL"  
295 "1-OXYL"  
( "1" (W) "OXYL" )  
L22 69 "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

=> d l22, all

L22 ANSWER 1 OF 69 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 347362-24-7 REGISTRY  
ED Entered STN: 23 Jul 2001  
CN 1-Piperidinyloxy, 4-[(9-anthracenylcarbonyl)oxy]-2,2,6,6-tetramethyl-  
(9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 4-(9-Anthroyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl

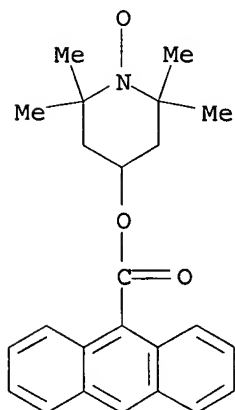
Updated Search

10509228

MF C24 H26 N O3  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Journal  
RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation);  
PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES  
(Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N	NC5	6	C5N	46.156.1	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2508.17.56	1



4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 136:199849 CA  
TI Anthracene Derivatives and the Corresponding Dimers with TEMPO Radicals  
AU Nakatsuji, Shin'ichi; Ojima, Takeo; Akutsu, Hiroki; Yamada, Junichi  
CS Department of Material Science Faculty of Science, Himeji Institute of  
Technology, Kamigori, Hyogo, 678-1297, Japan  
SO Journal of Organic Chemistry (2002), 67(3), 916-921  
CODEN: JOCEAH; ISSN: 0022-3263  
PB American Chemical Society  
DT Journal  
LA English  
CC 22-5 (Physical Organic Chemistry)  
Section cross-reference(s): 74, 77  
AB Anthracene derivs. with several TEMPO radicals 9-C14H9-X-TEMPO where X is  
a linker from the 9 position of anthracene to the 4 position of TEMPO [X =  
CONH, CONMe, CO2, CH2NH (2, 3, 4, and 10, resp.)] were prepared, and each  
photodimerization reaction was investigated. Although the

Updated Search

photodimerization was unsuccessful in obtaining the dimers of anthracenes 2 and 3, which could be alternatively prepared in a stepwise manner, the photodimers (all photodimers trans in this abstract) of anthracenes 4 and 10 were available by the direct photoreaction. The dissociation reaction of the dimers proceeded well by heating them in solution to give the corresponding monomers in each case, and thus the reversible system could be constructed in the latter two systems. While no large difference was observed in their magnetic behaviors between the monomer/dimer pair of monomer 4 and dimer 8, an intriguing difference was found in the magnetic behaviors for the pair of monomer 10 and dimer 11 from ferromagnetic interactions in 10 to the variable magnetic interactions in 11 depending on the solvent mols. incorporated in the crystals.

- ST anthracene TEMPO deriv photodimerization magnetic property
- IT Hydrogen bond  
(ferromagnetic coupling through hydrogen bonds; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Dimerization  
(photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Antiferromagnetic exchange  
Configuration  
Curie-Weiss law  
ESR (electron spin resonance)  
Exchange interaction  
Ferromagnetic exchange  
Magnetic susceptibility  
Solvates  
Zero field splitting  
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Nitroxides  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Clathrates  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Ring opening  
(thermal; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 14691-88-4, 4-Amino-TEMPO  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(amidation and reductive amination; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 723-62-6, 9-Anthracenecarboxylic acid 108654-32-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(amidation; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 42585-33-1P, 4-(Methylamino)-TEMPO  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(amidation; preparation and reversible photodimerization of anthracene TEMPO

- derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 363148-79-2P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (attempted direct photodimerization, crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-23-6P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (attempted direct photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-91-0P 295797-93-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-89-6P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (direct photodimerization, crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-24-7P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (direct photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-92-1P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 2226-96-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-25-8P 401796-52-9P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation from 9-anthracenecarboxylic acid photodimer; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 150809-84-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (reduction; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 642-31-9, 9-Anthraldehyde 2896-70-0, 4-Oxo-TEMPO  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reductive amination; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-90-9P 347362-26-9P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (thermal cycloreversion; preparation and reversible photodimerization of

anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (2) Akutsu, H; Synth Met 2001, V120, P871 CAPLUS
- (3) Bouas-Laurent, H; Chem Soc Rev 2000, V29, P43 CAPLUS
- (4) Cowan, D; J Am Chem Soc 1972, V94, P6779 CAPLUS
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# REFERENCE 2

AN 136:47590 CA  
 TI Investigation of the anthracene-nitroxide hybrid molecule as a probe for hydroxyl radicals  
 AU Yang, Xiao-Feng; Guo, Xiang-Qun  
 CS Department of Chemistry and the Key Laboratory of Analytical Sciences of MOE, Xiamen University, Xiamen, 361005, Peop. Rep. China  
 SO Analyst (Cambridge, United Kingdom) (2001), 126(10), 1800-1804  
 CODEN: ANALAO; ISSN: 0003-2654  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 CC 79-3 (Inorganic Analytical Chemistry)  
 AB A new method for the determination of hydroxyl radicals is proposed. The method is based on the use of a hybrid mol. consisting of a fluorescent chromophore, anthracene, and a nitroxide radical. In the hybrid mol., the nitroxide quenches the fluorescence of anthracene strongly. The reaction of hydroxyl radicals with DMSO generates quant. Me radicals, which then combine with the nitroxide moiety of the hybrid mols. to result in an increase in the fluorescence intensity. The fluorescence increase is

proportional to the concentration of hydroxyl radicals. The proposed method is capable of detecting hydroxyl radicals generated in the Fenton system. It is a simple and sensitive technique for the determination of hydroxyl radicals.

ST anthracene nitroxide hybrid mol hydroxyl radical

IT Absorption spectra

Chromophores

Fenton reaction

Fluorescence

Fluorometry

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 3352-57-6, Hydroxyl, analysis 380202-05-1

RL: ANT (Analyte); ANST (Analytical study)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 347362-24-7P, 4-(9-Anthroxyl)-2,2,6,6-tetramethylpiperidine-1-oxyl

RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST (Analytical study); PREP (Preparation); USES (Uses)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 723-62-6, 9-Anthracenecarboxylic acid 2226-96-2,

4-Hydroxy-2,2,6,6-tetramethylpiperidinyloxyl

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 16331-52-5P, 9-Anthracenecarboxylic acid chloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 67-68-5, DMSO, uses

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(hydroxyl trapping agent; hydroxyl radical determination by fluorometry

using

anthracene linked to TEMPO as fluorescent chromophore)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

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## REFERENCE 3

- AN 135:272668 CA
- TI Magnetic properties of anthracene derivatives and the corresponding photo-dimers with stable radical substituents
- AU Ojima, T.; Akutsu, H.; Yamada, J.-i.; Nakatsuji, S.
- CS Faculty of Science, Department of Material Science, Himeji Institute of Technology, Kamigori, Hyogo, 678-1297, Japan
- SO Polyhedron (2001), 20(11-14), 1335-1338  
CODEN: PLYHDE; ISSN: 0277-5387
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- CC 22-13 (Physical Organic Chemistry)  
Section cross-reference(s): 75, 77
- AB Several anthracene derivs. with stable radical substituents have been prepared and their magnetic properties have been investigated together with those of some of the dimers available by photo-dimerization reaction. While weak magnetic interactions with Curie-Weiss behavior have been observed in most derivs. prepared, antiferromagnetic behavior being based on an S-T model has been found in the spins of TEMPO-substituted N-methylcarboxyamidoanthracene derivative 1c. The magnetic property of Mn(hfac)<sub>2</sub> complex derived from 4-amino-TEMPO-substituted 9-methylanthracene (1d) is also described.
- ST TEMPO substituted magnetic property crystallog
- IT Antiferromagnetism  
Crystal structure  
Curie-Weiss law  
Magnetic properties  
Magnetic susceptibility  
Molecular structure  
(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)
- IT Nitroxides  
RL: PRP (Properties)  
(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)
- IT 178170-34-8 295797-89-6 295797-90-9 347362-23-6 347362-24-7  
347362-25-8 347362-26-9 363148-79-2 363158-33-2  
RL: PRP (Properties)

(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Caneschi, A; Inorg Chem 1988, V27, P2027 CAPLUS.
- (2) Dickman, M; Inorg Chem 1986, V25, P2595 CAPLUS
- (3) Gutlich, P; Angew Chem Int Ed 1994, V33, P2024
- (4) Hamachi, K; Bull Chem Soc 1998, V71, P2937 CAPLUS
- (5) Matsuda, K; Chem Lett 2000, P16 CAPLUS
- (6) Matsuda, K; J Am Chem Soc 2000, V122, P7195 CAPLUS
- (7) Matsuda, K; J Am Chem Soc 2000, V122, P8309 CAPLUS
- (8) Matsuda, K; Tetrahedron Lett 2000, V41, P2577 CAPLUS
- (9) Nagai, K; Solid State Commun 1997, V102, P809 CAPLUS
- (10) Nakatsuji, S; J Chem Soc, Perkin Trans 2 2000, P1969 CAPLUS
- (11) Nakatsuji, S; Mol Cryst Liq Cryst 1996, V279, P73 CAPLUS
- (12) Nakatsuji, S; Mol Cryst Liq Cryst 2000, V348, P1 CAPLUS
- (13) Nakatsuji, S; Mol Cryst Liq Cryst in press 2001
- (14) Nakatsuji, S; Mol Cryst Liq Cryst in press 2001
- (15) Ojima, T; Chem Lett 2000, P918 CAPLUS
- (16) Sato, O; Science 1996, V272, P704 CAPLUS
- (17) Takeuchi, S; Mol Cryst Liq Cryst 2000, V345, P167 CAPLUS
- (18) Verdaguer, M; Science 1996, V272, P698 CAPLUS

#### REFERENCE 4

- AN 135:84149 CA
- TI Preparation and properties of photofunctional systems with nitroxide radicals
- AU Nakatsuji, Shin'ichi; Takeuchi, Soichi; Ojima, Takeo; Ogawa, Yuya; Akutsu, Hiroki; Yamada, Jun-Ichi
- CS Department of Material Science, Faculty of Science, Himeji Institute of Technology, Kamigori, 678-1297, Japan
- SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2001), 356, 23-32  
CODEN: MCLCE9; ISSN: 1058-725X
- PB Gordon & Breach Science Publishers
- DT Journal
- LA English
- CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
Section cross-reference(s): 77
- AB Series of TEMPO-substituted norbornadiene, spiropyran and anthracene derivs. have been prepared: their light-induced structural change to the corresponding quadricyclanes, merocyanines or anthracene-dimers and the reverse reactions to the starting materials have been studied. The antiferromagnetic or ferromagnetic behavior observed in norbornadienes/anthracenes was found to be preserved in the corresponding quadricyclanes/anthracene-dimers in spite of the difference of their Weiss temps., whereas switching of the intermol. magnetic interactions was observed in spiropyran/merocyanine systems.
- ST photofunctional organomagnēt nitroxide radical substituted mol photoreaction; norbornadiene piperidyloxy substituted org photoreactive mol magnetic property; spiropyran piperidyloxy substituted org photoreactive mol magnetic property; anthracene piperidyloxy substituted org photoreactive mol magnetic property
- IT Ring opening  
(photochem.; photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnēt system)
- IT Dimerization



- (photodimerization; photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT Antiferromagnetic materials  
Curie-Weiss law  
Ferromagnetic materials  
Magnetic properties  
Magnetic susceptibility  
Photolysis  
(photofunctional organomagnets including methylpiperidyloxy-substituted norbornadiene- and spiropyran- and anthracene derivs.)
- IT Isomerization  
(valence, photochem.; photoinduced reversible reactions and properties of methylpiperidyloxy-substituted norbornadiene derivative photofunctional organomagnets)
- IT 347362-25-8 347362-26-9  
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT 347362-21-4 347362-22-5 347362-23-6 347362-24-7  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT 307307-48-8P 307307-49-9P 307307-50-2P  
RL: FMU (Formation, unclassified); PNU (Preparation, unclassified); PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted norbornadiene derivative/ qudricyclane photofunctional organomagnet system)
- IT 307307-45-5P 307307-46-6P 307307-47-7P  
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); PROC (Process)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted norbornadiene derivative/ qudricyclane photofunctional organomagnet system)
- IT 347362-29-2 347362-30-5  
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnet system)
- IT 347362-27-0 347362-28-1  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnet system)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Cowan, D; J Am Chem Soc 1972, V94, P6779 CAPLUS
- (2) Cristol, S; J Am Chem Soc 1958, V80, P1950 CAPLUS
- (3) Guglielmetti, R; Photochromism: Molecules and Systems 1990
- (4) Gutlich, P; Angew, Chem Int Ed 1994, V33, P2024
- (5) Hamachi, K; Bull Chem Soc 1998, V71, P2937 CAPLUS

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- (6) Hassner, A; Tetrahedron Lett 1978, V46, P4475
- (7) Hautala, R; Solar Energy Chemical Conversion and Storage 1979
- (8) Matsuda, K; the Annual Meeting of Chemical Society of Japan held in Yokohama 1999, 3G2 16, P404
- (9) Nagai, K; Solid State Commun 1997, V102, P809 CAPLUS
- (10) Nakatsuji, S; New J Chem 1998, P275 CAPLUS
- (11) Namba, K; Bull Chem Soc 1975, V48, P1323 CAPLUS
- (12) Natatsuji, S; J Mater Chem 1997, V7, P2161
- (13) Sato, O; Science 1996, V272, P704 CAPLUS
- (14) Schonberg, A; Preparative Organic Photochemistry 1968
- (15) Verdaguer, M; Science 1996, V272, P698 CAPLUS

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006  
SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
44.62	98.00

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.71	-0.71

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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16  
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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L23 7022 L21

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L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON  
L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006  
L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006  
L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

Updated Search

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FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006  
SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006  
L23 7022 S L21

=> s l23 and l11  
L24 1 L23 AND L11

=> d l24, ibib abs hitstr, 1

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:213306 HCAPLUS

DOCUMENT NUMBER: 140:253453

TITLE: Process for the preparation of 1,3-dihydro-6-methylfuro(3,4-c)pyridin-7-ol derivatives, in particular cicletanine hydrochloride, by protection, oxidation, addition of a nucleophile, and one pot deprotection/cyclodehydration

INVENTOR(S): Gore, Vinayak G.; Ghadge, Manoj M.; Gupta, Ashwini Kumar K.

PATENT ASSIGNEE(S): Generics (UK) Limited, UK

SOURCE: Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

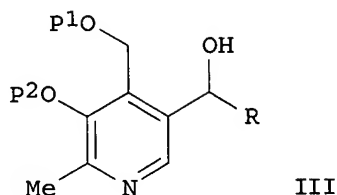
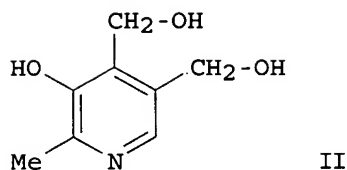
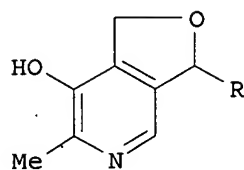
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398316	A2	20040317	EP 2003-255795	20030916
EP 1398316	A3	20040414		
EP 1398316	B1	20060614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 329918	E	20060715	AT 2003-255795	20030916
PRIORITY APPLN. INFO.:			GB 2002-21494	A 20020916
OTHER SOURCE(S):	CASREACT 140:253453; MARPAT 140:253453			
GI				



AB The invention is directed to the preparation of 1,3-dihydro-6-methylfuro(3,4-c)pyridin-7-ols I or salt by selective protection of pyridoxine II or salt, oxidation of the 3,4-protected pyridoxine with aqueous NaClO in the presence of catalytic amount of TEMPO, addition of a nucleophile, especially a Grignard reagent,

to the 3,4-protected pyridoxal, and one pot deprotection/cyclodehydration of III [R = substituted al(en/yn)yl, alkyl/alkenyl/alkynyl/aryl, arylalk(en/yn)yl which may include one or more N, O, or S; P1, P2 = independently protecting groups or together form one protecting group]. The invention is directed in particular to preparation of the well-known antihypertensive agent cicletanine hydrochloride (I•HCl, where R = 4-chlorophenyl). The advantages include environmentally friendly starting materials, simple process, and therefore an easy industrial scale-up. For example, cicletanine hydrochloride was prepared protection of pyridoxine hydrochloride with acetone/HCl, oxidation of the pyridinylmethyl alc. with NaClO in the presence of TEMPO/NaHCO3/DCM, addition of the 4-chlorophenylmagnesium bromide generated in situ from Mg and 4-bromochlorobenzene in THF at reflux, followed by one pot deprotection/cyclodehydration with concentrated HCl at reflux.

IT 6560-65-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(aldehyde intermediate; process for preparation of cicletanine hydrochloride and its derivs. by protection, oxidation, addition of a nucleophile, and one pot deprotection/cyclodehydration)

RN 6560-65-2 HCAPLUS

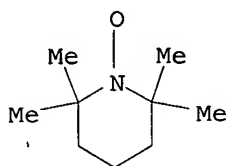
CN 4H-1,3-Dioxino[4,5-c]pyridine-5-carboxaldehyde, 2,2,8-trimethyl- (9CI)  
(CA INDEX NAME)

CN1C=CC2=C(C=C1)C(=O)OC(C2)C(C)(C)C

```

IT      2564-83-2, 2,2,6,6-Tetramethyl-1-piperidinyloxy
        RL: CAT (Catalyst use); USES (Uses)
            (catalyst; process for preparation of cicletanine hydrochloride and its
            derivs. by protection, oxidation, addition of a nucleophile, and one pot
            deprotection/cyclodehydration)
RN      2564-83-2 HCAPLUS
CN      1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
50.65	148.65
.	
SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-1.46

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006

SET POSTINGS ON  
L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON  
L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21  
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

=> s l11 and l22 and l8  
TOO MANY TERMS FOR FILE CROSSOVER IN L8  
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=> s l11 and l22  
TOO MANY TERMS FOR FILE CROSSOVER IN L8  
There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s l11 and l22  
TOO MANY TERMS FOR FILE CROSSOVER IN L8  
There are limits on the size of an answer set being crossed over from

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=> s l22

L25 59 L22

=> s l11

TOO MANY TERMS FOR FILE CROSSOVER IN L8

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=> s l11

TOO MANY TERMS FOR FILE CROSSOVER IN L8

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

2.20	150.85
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-1.46
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SET COMMAND COMPLETED

=> s "1-oxyl-4-yl" and tetramethyl and piperidine

19346742 "1"

7516 "OXYL"

17443241 "4"

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10509228

15372835 "YL"  
210 "YLS"  
15372835 "YL"  
("YL" OR "YLS")  
5 "1-OXYL-4-YL"  
("1" (W) "OXYL" (W) "4" (W) "YL")  
383162 TETRAMETHYL  
2 TETRAMETHYLS  
383162 TETRAMETHYL  
(TETRAMETHYL OR TETRAMETHYLS)  
394986 PIPERIDINE  
L26 1 "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE

=> d 126

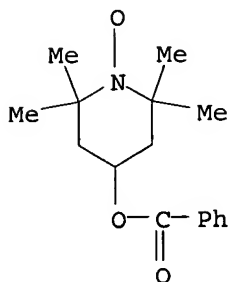
L26 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 3225-26-1 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA  
INDEX NAME)

OTHER CA INDEX NAMES:

CN Piperidinooxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)  
CN Piperidinooxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester)  
(8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate  
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine  
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl  
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate  
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxyl  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidinyl-1-oxyl benzoate  
CN Tempol benzoate  
MF C16 H22 N O3  
CI COM  
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
CHEMINFORMRX, CSCHEM, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)



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251 REFERENCES IN FILE CA (1907 TO DATE)  
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006

SET POSTINGS ON  
L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON  
L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21  
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006

SET POSTINGS ON  
L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE

=> s "2,2,6,6-tetramethyl" and piperidine and "1-oxyl-4-yl"

Updated Search

10509228

32058 "2,2,6,6"  
383162 "TETRAMETHYL"  
2 "TETRAMETHYLS"  
383162 "TETRAMETHYL"  
("TETRAMETHYL" OR "TETRAMETHYLS")  
30406 "2,2,6,6-TETRAMETHYL"  
("2,2,6,6" (W) "TETRAMETHYL")  
394986 PIPERIDINE  
19346742 "1"  
7516 "OXYL"  
17443241 "4"  
15372835 "YL"  
210 "YLS"  
15372835 "YL"  
("YL" OR "YLS")  
5 "1-OXYL-4-YL"  
("1" (W) "OXYL" (W) "4" (W) "YL")  
L27 1 "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

=>. d 127

L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 3225-26-1 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA  
INDEX NAME)

OTHER CA INDEX NAMES:

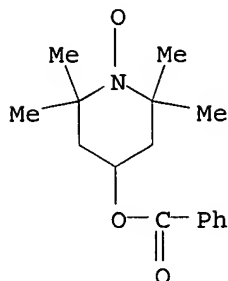
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)  
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester)  
(8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate  
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine  
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl  
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate  
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxy  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidinyl-1-oxyl benzoate  
CN Tempol benzoate  
MF C16 H22 N O3  
CI COM  
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
CHEMINFORMRX, CSCHEM, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)

Updated Search

10509228



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

251 REFERENCES IN FILE CA (1907 TO DATE)  
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

Updated Search

10509228

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006  
L23 7022 S L21  
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006  
L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006  
SET POSTINGS ON  
L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE  
L27 1 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

=> file hcaplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
67.00	217.85

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.46

CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 17:50:43 ON 12 OCT 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16  
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l27  
L28 251 L27

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006  
L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006  
SET POSTINGS ON

Updated Search

10509228

L4 0 S HETEROCYCLIC AND ALDEHYDE  
L5 296422 S ALDEHYDE?  
L6 2 S HETEROCYCLIC  
L7 0 S L6 AND L5  
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP  
L10 100866 S L8/RCT  
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?  
L13 0 S L12 () L11  
L14 0 S L12 AND L11  
L15 166106 S HALOGEN?  
L16 28 S L15 () L11  
L17 0 S L12 (L) L11  
L18 0 S L12 AND L11  
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE  
L21 92 S L20 AND OXYL  
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21  
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006

SET POSTINGS ON

L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE  
L27 1 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

FILE 'HCAPLUS' ENTERED AT 17:50:43 ON 12 OCT 2006

L28 251 S L27

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.53	220.38

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.46

CA SUBSCRIBER PRICE

FILE 'CAOLD' ENTERED AT 17:50:57 ON 12 OCT 2006  
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

Updated Search

10509228

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l27 and l25

2 L27  
L29 2 L27 AND L25

=> d l29, all, 1-2

L29 ANSWER 1 OF 2 CAOLD COPYRIGHT 2006 ACS on STN  
AN CA65:10559e CAOLD  
TI synthesis of heterocyclic analogs of hydroxylamine  
AU Rozantsev, E. G.; Golubev, V. A.  
IT 768-66-1 850-43-1 3225-26-1 3637-10-3 3637-11-4  
4972-13-8 7031-85-8 7031-86-9 7031-87-0 7031-88-1 7031-89-2  
7031-90-5 7031-92-7 7031-93-8 7031-94-9 7031-95-0 7031-96-1  
7032-00-0 7032-01-1 7166-32-7 10439-48-2 16203-28-4  
  
L29 ANSWER 2 OF 2 CAOLD COPYRIGHT 2006 ACS on STN  
AN CA62:14621b CAOLD  
TI free radicals in iminoxyl series in the group of hydrogenated pyridine  
AU Rozantsev, E. G.; Golubev, V. A.; Neiman, M. B.  
TI preparation of N-tert-butyl-4-piperidone  
AU Robinson, John Barry; Thomas, J.  
IT 1462-98-2 1462-99-3 1463-00-9 1465-76-5 1742-82-1 1796-15-2  
1796-16-3 1796-17-4 1796-18-5 1796-19-6 1796-20-9 2013-75-4  
2234-55-1 3225-24-9 3225-25-0 3225-26-1 3225-27-2  
3264-93-5

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	1.78	222.16
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.46

FILE 'REGISTRY' ENTERED AT 17:51:21 ON 12 OCT 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

Updated Search

10509228

DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 3225-26-1/RN

L30 1 3225-26-1/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L30 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L30 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 3225-26-1 REGISTRY  
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA INDEX  
NAME)

OTHER CA INDEX NAMES:

CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)  
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester) (8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate  
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine  
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl  
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide  
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate  
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate  
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxy  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl  
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate  
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidiny-1-oxyl benzoate  
CN Tempol benzoate

MF C16 H22 N O3

CI COM

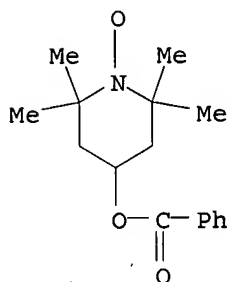
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
CHEMINFORMRX, CSCHM, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL

Updated Search



10509228

(\*File contains numerically searchable property data)  
DT.CA Caplus document type: Conference; Journal; Patent  
RL.P Roles from patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)  
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)  
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)  
RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

251 REFERENCES IN FILE CA (1907 TO DATE)  
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

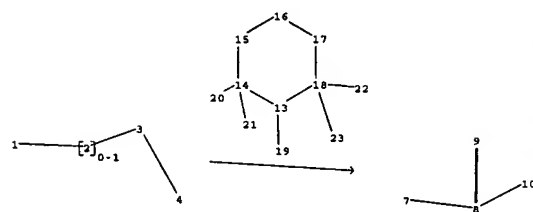
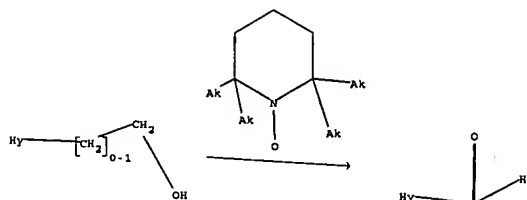
=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

=>

Updated Search



chain nodes :

1 2 3 4 7 8 9 10 19 20 21 22 23

ring nodes :

13 14 15 16 17 18

chain bonds :

1-2 2-3 3-4 7-8 8-9 8-10 13-19 14-20 14-21 18-22 18-23

ring bonds :

13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-2 7-8 8-9 13-14 13-18 13-19 14-15 14-20 14-21 15-16 16-17 17-18 18-22 18-23

exact bonds :

2-3 3-4 8-10

isolated ring systems :

containing 13 :

Match level :

1:Atom 2:CLASS3:CLASS4:CLASS7:Atom 8:CLASS9:CLASS10:CLASS13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS

fragments assigned reactant role:

containing 1

fragments assigned reagent role:

containing 13

fragments assigned product role:



10509228

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal612bxr

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	4	MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS	5	MAY 11	KOREAPAT updates resume
NEWS	6	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS	7	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPATFULL/USPAT2
NEWS	8	MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS	9	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS	10	JUN 26	TULSA/TULSA2 reloaded and enhanced with new search and and display fields
NEWS	11	JUN 28	Price changes in full-text patent databases EPFULL and PCTFULL
NEWS	12	JUL 11	CHEMSAFE reloaded and enhanced
NEWS	13	JUL 14	FSTA enhanced with Japanese patents
NEWS	14	JUL 19	Coverage of Research Disclosure reinstated in DWPI
NEWS	15	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	16	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	17	AUG 30	CA(SM)/CAPLUS(SM) Austrian patent law changes
NEWS	18	SEP 11	CA/CAPLUS enhanced with more pre-1907 records
NEWS	19	SEP 21	CA/CAPLUS fields enhanced with simultaneous left and right truncation
NEWS	20	SEP 25	CA(SM)/CAPLUS(SM) display of CA Lexicon enhanced
NEWS	21	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	22	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	23	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that  
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10509228

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

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FILE CONTENT:1840 - 8 Oct 2006 VOL 145 ISS 15

New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\* CASREACT now has more than 10 million reactions \*  
\* \*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\oioi.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 19:54:15 FILE 'CASREACT'

SCREENING COMPLETE - 6029 REACTIONS TO VERIFY FROM

147 DOCUMENTS

82.9% DONE 5000 VERIFIED 12 HIT RXNS

3 DOCS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 115946 TO 125214

PROJECTED ANSWERS: 3 TO 213

L2 3 SEA SSS SAM L1 ( 12 REACTIONS)

Updated Search

10509228

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 109.70 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y

FULL SEARCH INITIATED 19:54:20 FILE 'CASREACT'

SCREENING COMPLETE - 119561 REACTIONS TO VERIFY FROM 3061 DOCUMENTS

100.0% DONE 119561 VERIFIED 131 HIT RXNS 38 DOCS

SEARCH TIME: 00.00.05

L3 38 SEA SSS FUL L1 ( 131 REACTIONS)

=> s l3 and shiomi, y?/au

18 SHIOMI, Y?/AU

L4 0 L3 AND SHIOMI, Y?/AU

=> s l3 and uno, o?/au

9 UNO, O?/AU

L5 0 L3 AND UNO, O?/AU

=> s l3 and ohta, a?/au

89 OHTA, A?/AU

L6 0 L3 AND OHTA, A?/AU

=> s l3 and sunakami, t?/au

0 SUNAKAMI, T?/AU

L7 0 L3 AND SUNAKAMI, T?/AU

=> d l3, ibib abs hit, 1-38

L3 ANSWER 1 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 145:64877 CASREACT

TITLE: Conversion of 2,5-(hydroxymethyl)furaldehyde to industrial derivatives, purification of the derivatives, and industrial uses therefor

INVENTOR(S): Sanborn, Alexandra, J.; Bloom, Paul, D.

PATENT ASSIGNEE(S): Archer-Daniels-Midland Company, USA

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006063287	A2	20060615	WO 2005-US44721	20051209
WO 2006063287	A3	20060914		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

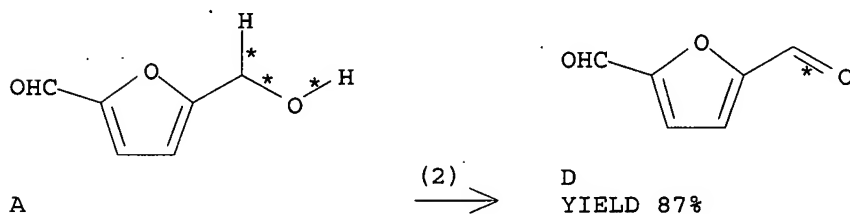
Updated Search

10509228

KG, KZ, MD, RU, TJ, TM  
 US 2006128843 A1 20060615 US 2005-70063 20050302  
 US 2006128977 A1 20060615 US 2005-273947 20051115  
 US 2006128844 A1 20060615 US 2005-274554 20051115  
 US 2006142599 A1 20060629 US 2005-298014 20051209  
 PRIORITY APPLN. INFO.: US 2004-635406P 20041210  
 US 2005-70063 20050302

AB A method of preparing 2,5-bis(hydroxymethyl)tetrahydrofuran comprises heating a reaction mixture comprising 2,5-(hydroxymethyl)furaldehyde, an organic solvent, and a catalyst system comprising nickel and zirconium at a temperature, for a time, and at a pressure sufficient to promote reduction of the 2,5-(hydroxymethyl)furaldehyde to 2,5-bis(hydroxymethyl)tetrahydrofuran to produce a product mixture comprising 2,5-bis(hydroxymethyl)tetrahydrofuran. 2,5-Furandialdehyde is also prepared 2,5-Bis(hydroxymethyl)tetrahydrofuran is useful in coatings.

RX(2) OF 2 A ==> D



RX(2) RCT A 67-47-0  
 RGT E 2564-83-2 Me4-piperidoxyl, F 3240-34-4 PhI(OAc)2  
 PRO D 823-82-5  
 SOL 108-10-1 i-BuCOMe  
 CON 1.5 hours, room temperature  
 NTE optimization study

L3 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 144:232853 CASREACT  
 TITLE: A process for the preparation of rosuvastatin involving a TEMPO-mediated oxidation step  
 INVENTOR(S): Niddam-Hildesheim, Valerie; Chen, Kobi  
 PATENT ASSIGNEE(S): Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals USA, Inc.  
 SOURCE: PCT Int. Appl., 25 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006017357	A1	20060216	WO 2005-US24983	20050713
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,				

Updated Search

10509228

LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,  
NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,  
SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,  
ZA, ZM, ZW  
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,  
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,  
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
KG, KZ, MD, RU, TJ, TM

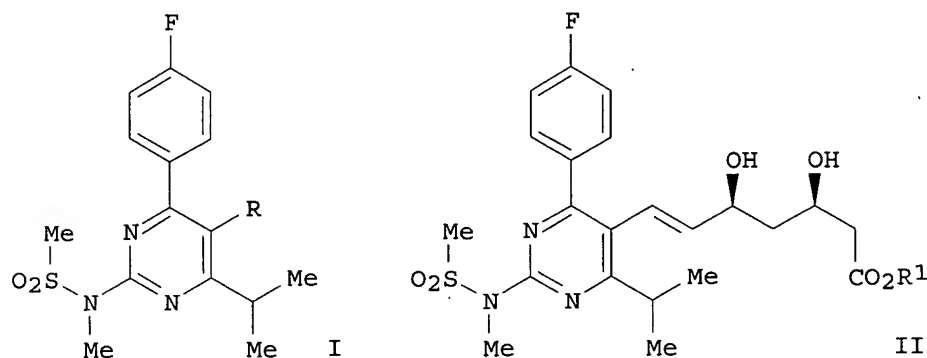
US 2006089501 A1 20060427 US 2005-181968 20050713  
EP 1673351 A1 20060628 EP 2005-771256 20050713

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK,  
BA, HR, IS, YU

PRIORITY APPLN. INFO.:

US 2004-587653P 20040713  
WO 2005-US24983 20050713

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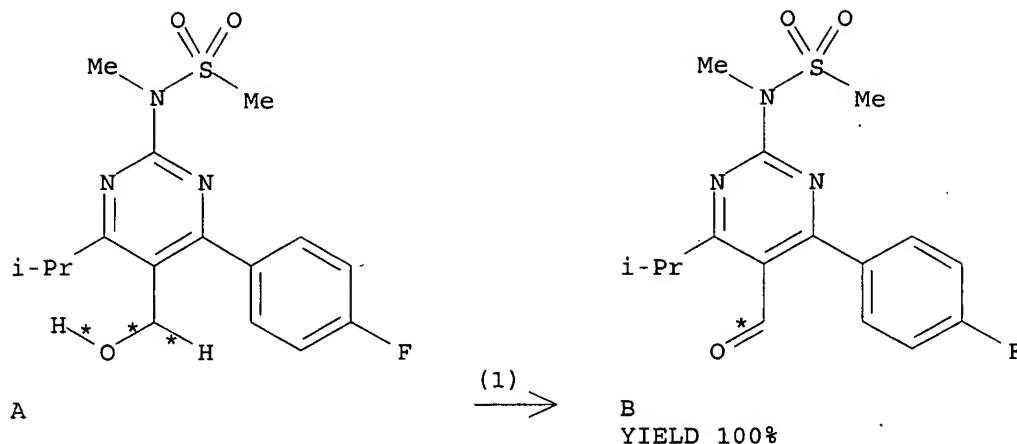


AB This invention provides a process for the preparation of the rosuvastatin intermediate I (R = CHO) by TEMPO-mediated oxidation of the corresponding alc. I (R = CH<sub>2</sub>OH), and its subsequent conversion to rosuvastatin II (R<sub>1</sub> = H) and pharmaceutically acceptable salts thereof, such as II (R<sub>1</sub> = Na, 1/2Ca).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 11 A ==> B





RX(1) RCT A 147118-36-3  
 RGT C 2564-83-2 Me4-piperidoxyl, D 7681-52-9 NaOCl, E  
 7758-02-3 KBr  
 PRO B 147118-37-4  
 SOL 7732-18-5 Water, 75-05-8 MeCN  
 CON SUBSTAGE(1) 5 deg C  
 SUBSTAGE(3) 6 hours  
 NTE optimization study

L3 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:367114 CASREACT  
 TITLE: Total Synthesis of (-)-Kaitocephalin  
 AUTHOR(S): Kawasaki, Masanori; Shinada, Tetsuro; Hamada, Makoto;  
 Ohfune, Yasufumi  
 CORPORATE SOURCE: Graduate School of Science, Osaka City University,  
 Sugimoto, Sumiyoshi, Osaka, 558-8585, Japan  
 SOURCE: Organic Letters (2005), 7(19), 4165-4167  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

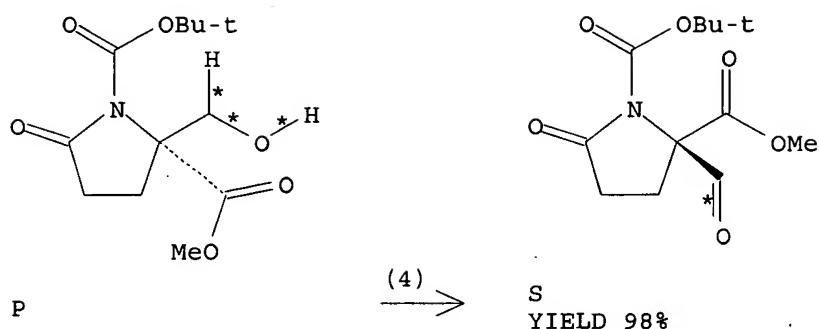
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Total synthesis of the potent AMPA/KA receptor antagonist  
 (-)-kaitocephalin (I) and its three diastereomers has been accomplished.  
 The synthesis features strictly substrate-controlled operations to  
 $\alpha$ -formylglutamate II starting with  $\alpha$ -hydroxymethylglutamate.  
 The requisite 2R,3S,7R-stereocenters were efficiently constructed by  
 manipulation of stereoselective reactions: dihydroxylation of III followed  
 by azide substitution of the corresponding thionocarbonate IV and  
 Cu-mediated allylation of an acyliminium ion. All of the protecting  
 groups in V were removed simultaneously by  $\text{AlCl}_3/\text{Me}_2\text{S}$  to give I.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10509228

RX(4) OF 464 ...P ==> S...



RX(4) RCT P 866331-68-2  
RGT T 2564-83-2 Me4-piperidoxyl, U 3240-34-4 PhI(OAc)2  
PRO S 866331-49-9  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 26 hours, room temperature

L3 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:326257 CASREACT

TITLE: Theoretical and Experimental Design of Atypical Kinase Inhibitors: Application to p38 MAP Kinase

AUTHOR(S): McClure, Kim F.; Abramov, Yuriy A.; Laird, Ellen R.; Barberia, John T.; Cai, Weiling; Carty, Thomas J.; Cortina, Santo R.; Danley, Dennis E.; Dipesa, Alan J.; Donahue, Kathleen M.; Dombroski, Mark A.; Elliott, Nancy C.; Gabel, Christopher A.; Han, Seungil; Hynes, Thomas R.; LeMotte, Peter K.; Mansour, Mahmoud N.; Marr, Eric S.; Letavic, Michaël A.; Pandit, Jayvardhan; Ripin, David B.; Sweeney, Francis J.; Tan, Douglas; Tao, Yong

CORPORATE SOURCE: Groton Laboratories, Pfizer Global Research and Development, Groton, CT, 06340, USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(18), 5728-5737

CODEN: JMCMAR; ISSN: 0022-2623

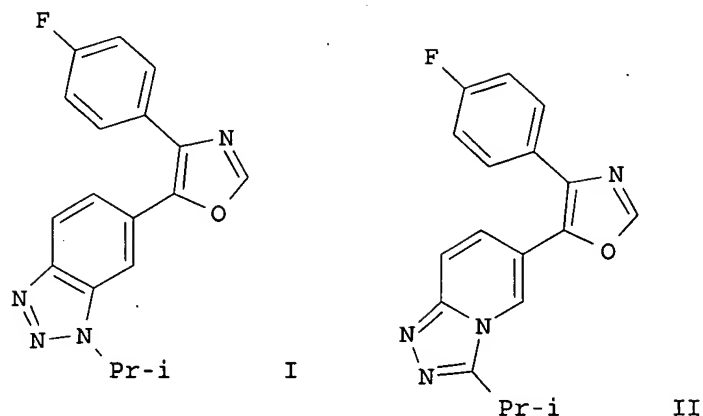
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

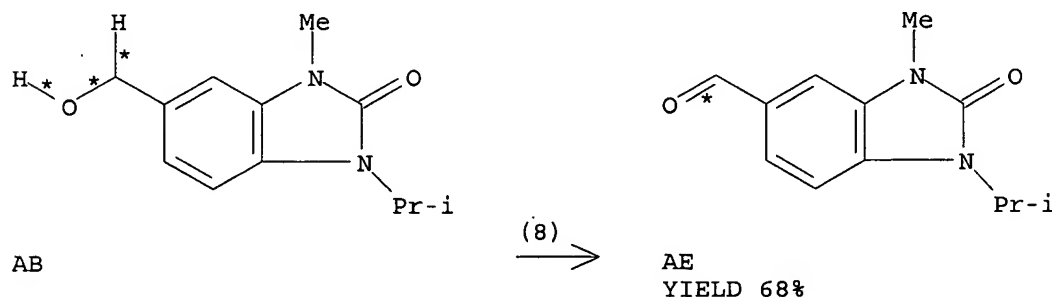
Updated Search



AB Mimics of the benzimidazolone nucleus found in inhibitors of p38 kinase are proposed, and their theor. potential as bioisosteres is described. A set of calculated descriptors relevant to the anticipated binding interaction for the fragments 1-methyl-1H-benzotriazole, 3-methylbenzo[d]isoxazole, and 3-methyl[1,2,4]triazolo[4,3-a]pyridine, pyridine, and 1,3-dimethyl-1,3-dihydro-benzoimidazol-2-one are reported. The design considerations and synthesis of p38 inhibitors based on these H-bond acceptor fragments is detailed. Comparative evaluation of the pyridine-, benzimidazolone-, benzotriazole-, and triazolopyridine-based inhibitors shows the triazoles I and II to be significantly more potent exptl. than the benzimidazolone after which they were modeled. An X-ray crystal structure of II bound to the active site shows that the triazole group serves as the H-bond acceptor but unexpectedly as a dual acceptor, inducing movement of the crossover connection of p38 $\alpha$ . The computed descriptors for the hydrophobic and  $\pi$ - $\pi$  interaction capacities were the most useful in ranking potency.

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(8) OF 71 ...AB ==> AE...



RX(8) RCT AB 865443-84-1  
 RGT AF 2564-83-2 Me4-piperidoxyl, AG 128-09-6  
 Chlorosuccinimide, AH 1112-67-0 Bu4NCl  
 PRO AE 865443-86-3  
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2

Updated Search

10509228

CON 18 hours, 22 deg C, pH 8.6  
NTE buffered solution, sodium bicarbonate-potassium carbonate

L3 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:229630 CASREACT

TITLE: Synthesis of Epoxyquinol A and Related Molecules:  
Probing Chemical Reactivity of Epoxyquinol Dimers and  
2H-Pyran Precursors

AUTHOR(S): Li, Chaomin; Porco, John A., Jr.

CORPORATE SOURCE: Department of Chemistry and Center for Chemical  
Methodology and Library Development, Boston  
University, Boston, MA, 02215, USA

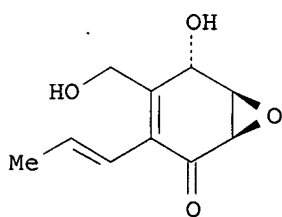
SOURCE: Journal of Organic Chemistry (2005), 70(15), 6053-6065  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

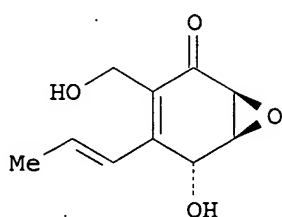
DOCUMENT TYPE: Journal

LANGUAGE: English

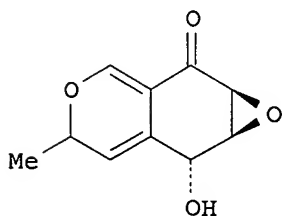
GI



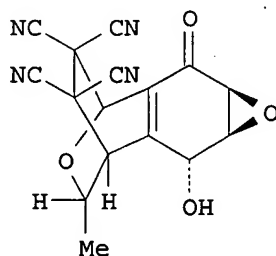
I



II



III



IV

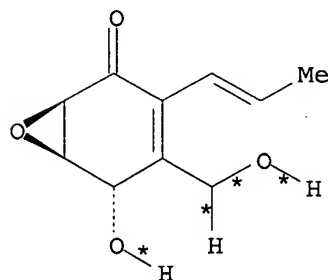
AB Total syntheses of the epoxyquinoid dimers, epoxyquinols A, B, and epoxytwinol A (RKB-3564 D), have been accomplished employing [4 + 2] and [4 + 4] dimerization of 2H-pyran epoxyquinol monomers, e.g. I. Modifications of 2H-pyran precursors have been explored, including alteration of epoxy alc. and diene stereochem. A stable 2H-pyran prepared by alteration of the epoxyquinol 2H-pyran nucleus was evaluated as a diene in Diels-Alder cycloaddn. with reactive dienophiles. Thus, reacting epoxyquinol II with Dess-Martin periodinane gave the 2H-pyran III which underwent Diels-Alder reaction with tetracyanoethylene to give adduct IV. Extensive studies for improving the [4 + 4] dimerization of selectively protected 2H-pyran monomers to afford the novel epoxyquinoid dimer epoxytwinol A were carried out, and valuable insight regarding competitive [4 + 2] and [4 + 4] dimerization processes has been obtained. In addition, chemical reactivities and structural modifications of epoxyquinol dimers have

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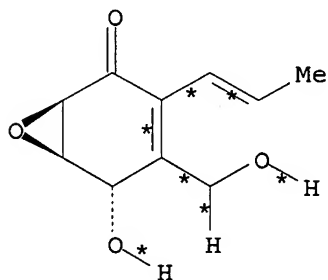
been evaluated, including [2 + 2] photocycloaddn. and [3,3] sigmatropic rearrangement, indicating the possibility for production of novel structural diversity from dimeric epoxyquinoid natural product frameworks.

REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

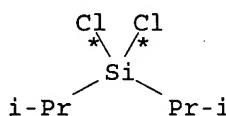
RX(25) OF 255 ...2 N + 2 BL ==> BM + BN...



N

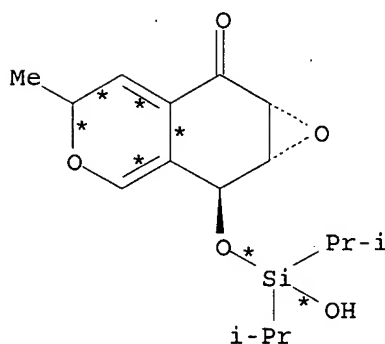


N

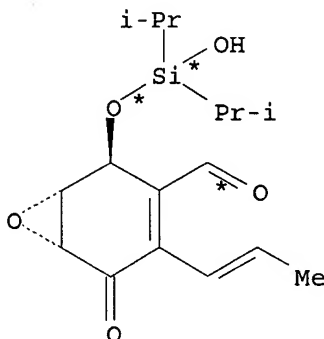


2 BL

(25)  
→



BM  
YIELD 76%



BN  
YIELD 15%

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me4-piperidoxyl, X 7782-44-7 O2, Y  
7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4  
RGT AY 288-32-4 1H-Imidazole  
SOL 68-12-2 DMF

Updated Search

10509228

CON 15 minutes, 0 deg C

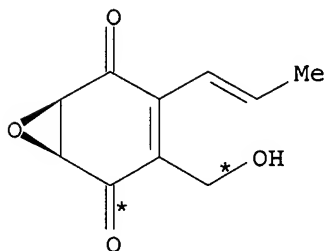
STAGE(3)

RGT L 7732-18-5 Water

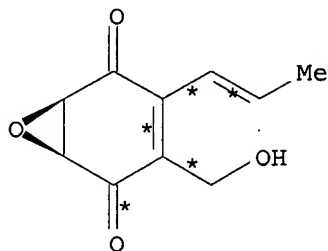
PRO BM 668987-33-5, BN 668987-32-4

RX(45) OF 255 COMPOSED OF RX(4), RX(25)

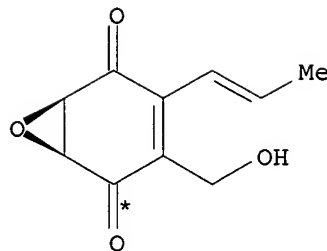
RX(45) 3 I + 2 BL ==> BM + BN



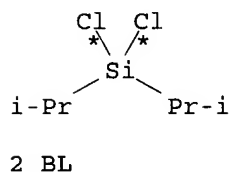
I



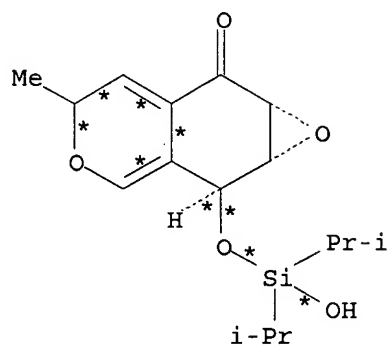
I



I

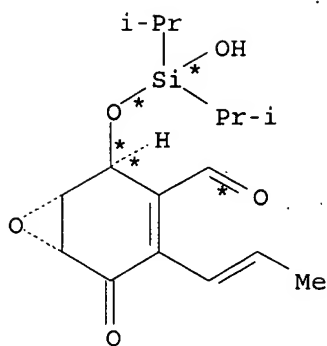


2  
STEPS  
→



BM  
YIELD 76%

10509228



BN  
YIELD 15%

RX(4) RCT I 473230-80-7

STAGE(1)

RGT P 1191-15-7 AlH(Bu-i)<sub>2</sub>  
SOL 109-99-9 THF, 110-54-3 Hexane  
CON SUBSTAGE(1) -78 deg C  
SUBSTAGE(2) 10 minutes, -78 deg C

STAGE(2)

RGT Q 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO N 238424-94-7, O 862593-54-2  
NTE stereoselective

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me<sub>4</sub>-piperidoxyl, X 7782-44-7 O<sub>2</sub>, Y  
7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4  
RGT AY 288-32-4 1H-Imidazole  
SOL 68-12-2 DMF  
CON 15 minutes, 0 deg C

STAGE(3)

RGT L 7732-18-5 Water

PRO BM 668987-33-5, BN 668987-32-4

L3 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:229621 CASREACT

TITLE: Stereoselective synthesis of microcarpalide

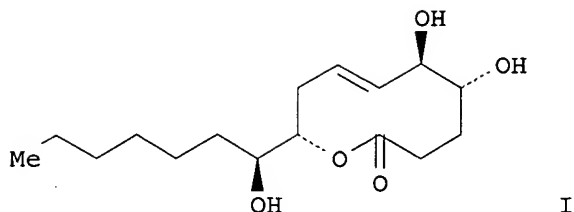
AUTHOR(S): Ishigami, Ken; Watanabe, Hidenori; Kitahara, Takeshi

CORPORATE SOURCE: Department of Applied Biological Chemistry, Graduate  
School of Agricultural and Life Sciences, The

Updated Search

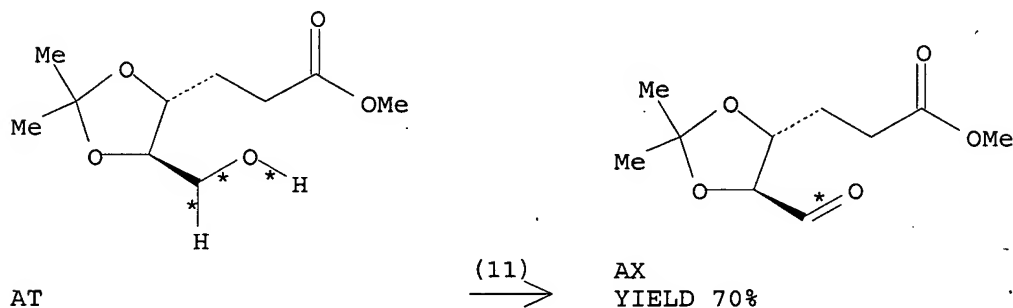
10509228

SOURCE: University of Tokyo, Bunkyo-ku, Tokyo, 113-8657, Japan  
Tetrahedron (2005), 61(31), 7546-7553  
CODEN: TETRAB; ISSN: 0040-4020  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Microcarpalide (I) is a strong microfilament disrupting agent. The convergent and stereoselective synthesis of microcarpalide was succeeded via Julia olefination and macrolactonization.  
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 171 ...AT ==> AX...



RX(11) RCT AT 850222-14-9

STAGE(1)

RGT AY 95407-69-5 1-Piperidinyloxy,  
4-methoxy-2,2,6,6-tetramethyl-, AZ 144-55-8 NaHCO<sub>3</sub>, BA  
7681-52-9 NaOCl, BB 7758-02-3 KBr  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 minutes, 0 deg C

STAGE(2)

RGT O 7772-98-7 Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>  
SOL 7732-18-5 Water

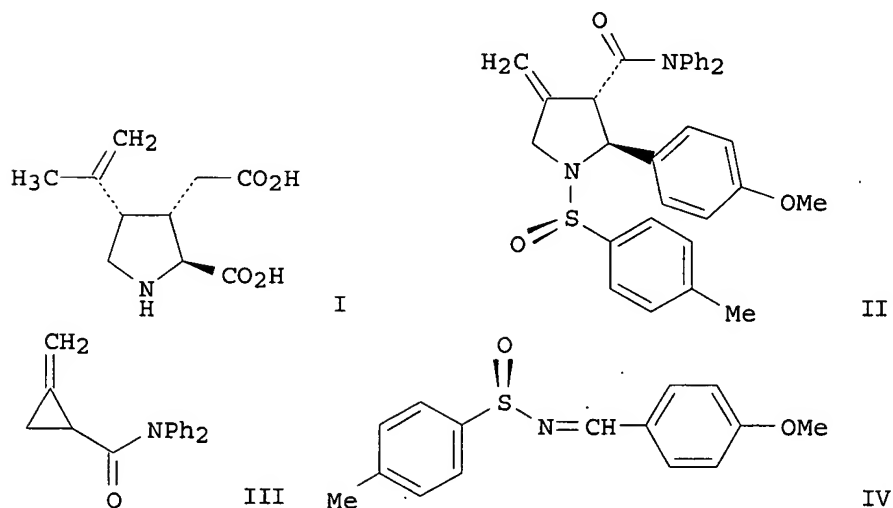
PRO AX 862907-39-9

Updated Search



10509228

L3 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 143:173109 CASREACT  
TITLE: Total Synthesis of (-)-( $\alpha$ )-Kainic Acid via a  
Diastereoselective Methylenecyclopropane Ring  
Expansion  
AUTHOR(S): Scott, Mark E.; Lautens, Mark  
CORPORATE SOURCE: Davenport Research Laboratories, Department of  
Chemistry, University of Toronto, Toronto, ON, M5S  
3H6, Can.  
SOURCE: Organic Letters (2005), 7(14), 3045-3047  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



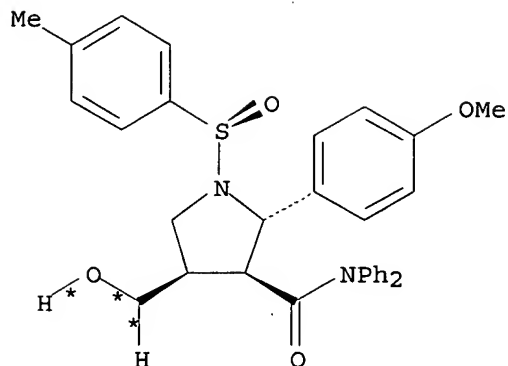
AB A concise and enantioselective synthesis of (-)- $\alpha$ -kainic acid (I) in 13 steps with an overall yield of 15% is reported. The kainoid precursor, (methylene)pyrrolidinyl amide II with the required C2/C3 trans stereochem., was prepared with excellent diastereoselectivity (>20:1) via a MgI<sub>2</sub>-mediated ring expansion of methylenecyclopropyl amide III with chiral sulfinimine IV. A selective hydroboration was then employed to set the remaining stereochem. at the C4 position en route to I.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

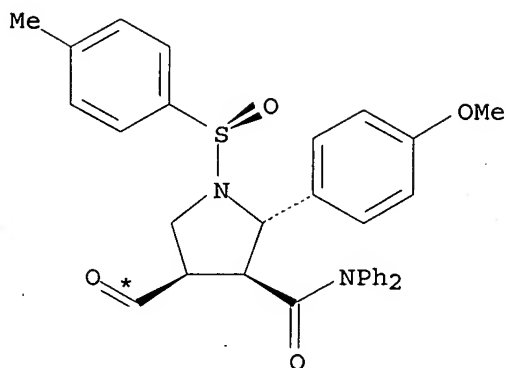
RX(3) OF 66 ...H ==> L...

Updated Search

10509228



H



L

YIELD 91%

RX(3) RCT H 861145-05-3

STAGE(1)

RGT M 2564-83-2 Me4-piperidoxyl, N 7647-15-6 NaBr  
SOL 7732-18-5 Water, 108-88-3 PhMe, 141-78-6 AcOEt  
CON room temperature -> 0 deg C

STAGE(2)

RGT O 144-55-8 NaHCO3, P 7681-52-9 NaOCl

PRO L 861145-06-4

L3 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:7520 CASREACT

TITLE: A total synthesis of the epoxyquinone based antifungal natural product (+)-ambuic acid

AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (2005), 46(17), 3045-3048

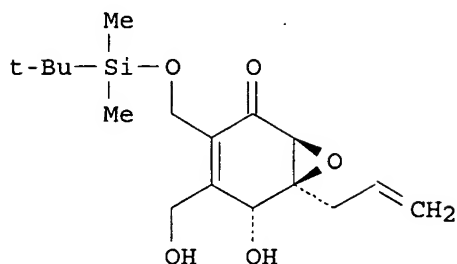
Updated Search

10509228

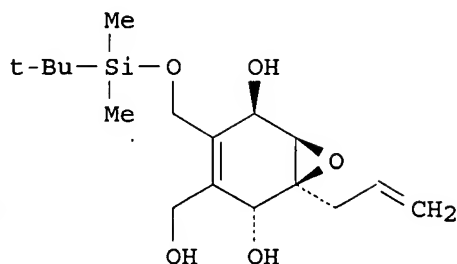
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:  
DOCUMENT TYPE:  
LANGUAGE:  
GI

Elsevier B.V.  
Journal  
English



I

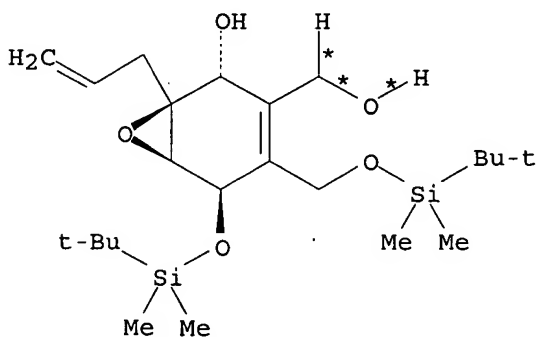


II

AB A total synthesis of the recently isolated polyketide natural product (+)-ambuic acid has been accomplished from the readily available Diels-Alder adduct of cyclopentadiene and 2-allyl-p-benzoquinone through a simple sequence with sound stereocontrol. An initial concern was to set the correct hydroxyl stereochem. at C7 in the evolution of epoxycyclohexanone I towards the natural product. This was accomplished by stereoselective NaBH<sub>4</sub> reduction of I with hydride addition from the face opposite to the epoxide ring which gave β-hydroxy compound II as the major product. II was then converted into the title compound

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

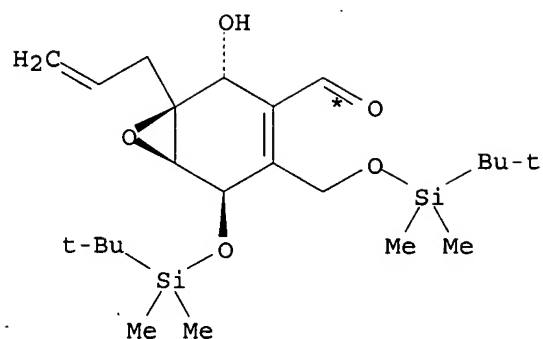
RX(5) OF 105 ...L ==> M...



L

(5) →

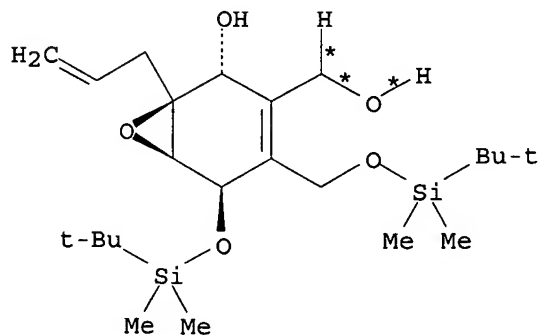
10509228



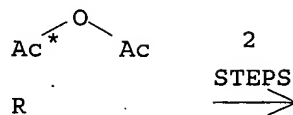
M  
YIELD 90%

RX(5) RCT L 852392-89-3  
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P  
7758-89-6 CuCl  
PRO M 852392-90-6  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

RX(19) OF 105 COMPOSED OF RX(5), RX(6)  
RX(19) L + R ==> S

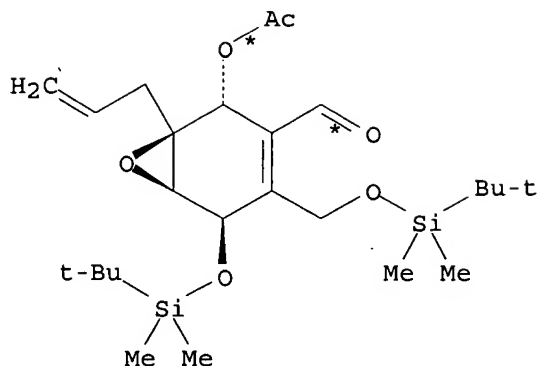


L



Updated Search

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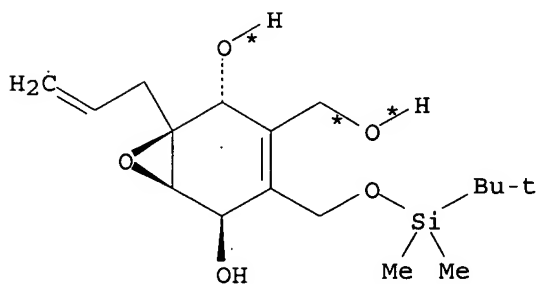


S  
YIELD 98%

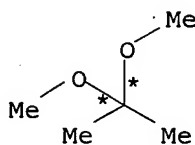
RX(5)     RCT   L 852392-89-3  
           RGT   N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P  
              7758-89-6 CuCl  
           PRO   M 852392-90-6  
           SOL   68-12-2 DMF  
           CON   3 hours, room temperature

RX(6)     RCT   M 852392-90-6, R 108-24-7  
           RGT   T 110-86-1 Pyridine, U 1122-58-3 4-DMAP  
           PRO   S 852392-91-7  
           SOL   75-09-2 CH2Cl2  
           CON   2.5 hours, 0 deg C

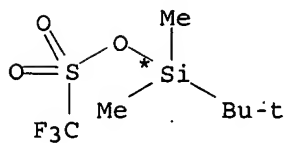
RX(32) OF 105 COMPOSED OF RX(2), RX(3), RX(4), RX(5)  
 RX(32)     B + E + H ==> M



B



E

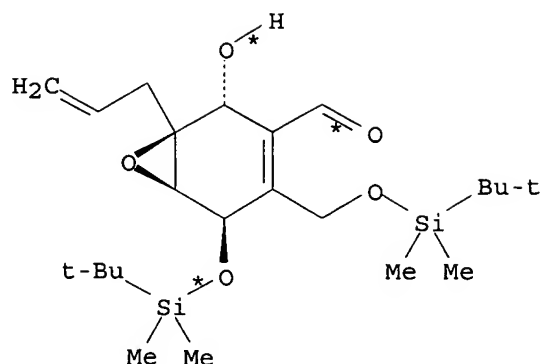


H

4  
STEPS  
→

Updated Search

10509228



M  
YIELD 90%

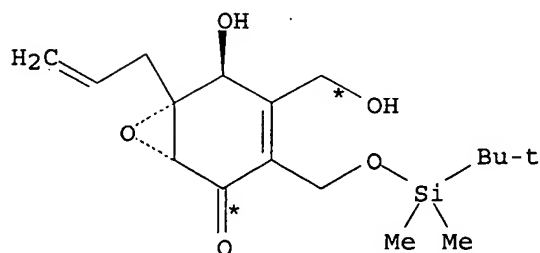
RX(2) RCT B 852392-86-0, E 77-76-9  
RGT G 24057-28-1 Pyridinium tosylate  
PRO F 852392-87-1  
CON 5 hours, room temperature

RX(3) RCT F 852392-87-1, H 69739-34-0  
RGT J 108-48-5 2,6-Lutidine  
PRO I 852392-88-2  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 minutes, 0 deg C

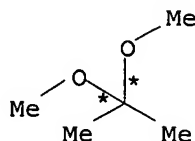
RX(4) RCT I 852392-88-2  
RGT G 24057-28-1 Pyridinium tosylate  
PRO L 852392-89-3  
SOL 67-56-1 MeOH  
CON 2 hours, room temperature

RX(5) RCT L 852392-89-3  
RGT N 2564-83-2 Me<sub>4</sub>-piperidoxyl, O 7782-44-7 O<sub>2</sub>, P 7758-89-6 CuCl  
PRO M 852392-90-6  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

RX(51) OF 105 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)  
RX(51) A + E + H ==> M



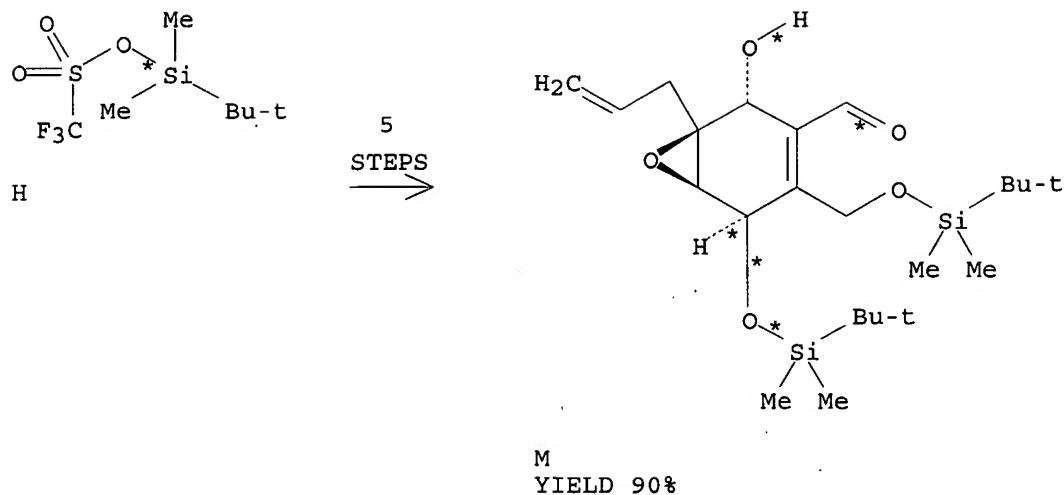
A



E

Updated Search

10509228

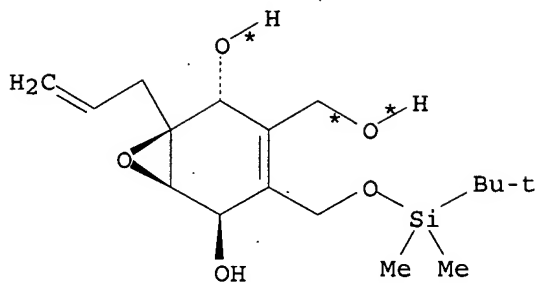


RX(1)	RCT	A 791854-39-2
	RGT	C 16940-66-2 NaBH4
	PRO	B 852392-86-0
	SOL	67-56-1 MeOH
	CON	10 minutes, -5 deg C
	NTE	stereoselective
RX(2)	RCT	B 852392-86-0, E 77-76-9
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	F 852392-87-1
	CON	5 hours, room temperature
RX(3)	RCT	F 852392-87-1, H 69739-34-0
	RGT	J 108-48-5 2,6-Lutidine
	PRO	I 852392-88-2
	SOL	75-09-2 CH2Cl2
	CON	15 minutes, 0 deg C
RX(4)	RCT	I 852392-88-2
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	L 852392-89-3
	SOL	67-56-1 MeOH
	CON	2 hours, room temperature
RX(5)	RCT	L 852392-89-3
	RGT	N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P 7758-89-6 CuCl
	PRO	M 852392-90-6
	SOL	68-12-2 DMF
	CON	3 hours, room temperature

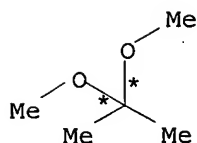
RX(52) OF 105 COMPOSED OF RX(2), RX(3), RX(4), RX(5), RX(6)  
 RX(52) B + E + H + R ==> S

Updated Search

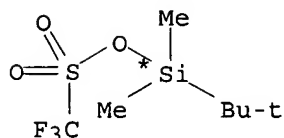
10509228



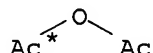
B



E

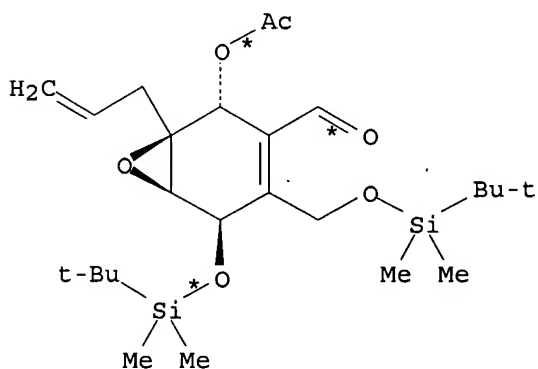


H



R

5  
STEPS  
→



S

YIELD 98%

RX(2)	RCT	B 852392-86-0, E 77-76-9
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	F 852392-87-1
	CON	5 hours, room temperature
RX(3)	RCT	F 852392-87-1, H 69739-34-0
	RGT	J 108-48-5 2,6-Lutidine
	PRO	I 852392-88-2
	SOL	75-09-2 CH2Cl2
	CON	15 minutes, 0 deg C
RX(4)	RCT	I 852392-88-2
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	L 852392-89-3

Updated Search



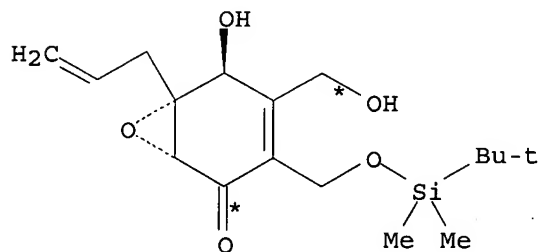
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SOL 67-56-1 MeOH  
CON 2 hours, room temperature

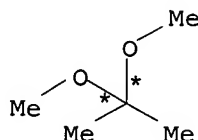
RX(5) RCT L 852392-89-3  
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P  
7758-89-6 CuCl  
PRO M 852392-90-6  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

RX(6) RCT M 852392-90-6, R 108-24-7  
RGT T 110-86-1 Pyridine, U 1122-58-3 4-DMAP  
PRO S 852392-91-7  
SOL 75-09-2 CH2Cl2  
CON 2.5 hours, 0 deg C

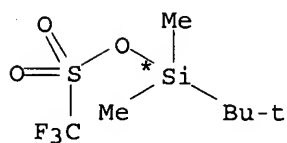
RX(53) OF 105 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)  
RX(53) A + E + H + R ==> S



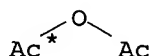
A



E



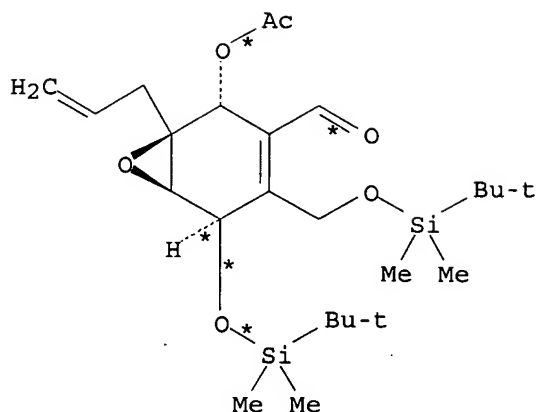
H



R

6  
STEPS  
→

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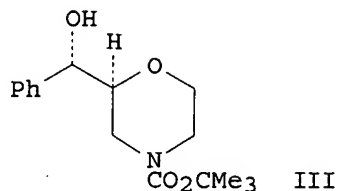
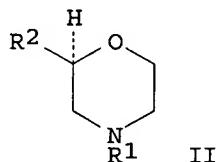
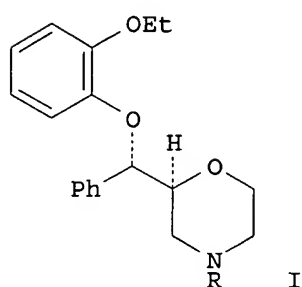
S  
YIELD 98%

RX(1)	RCT A 791854-39-2
	RGT C 16940-66-2 NaBH4
	PRO B 852392-86-0
	SOL 67-56-1 MeOH
	CON 10 minutes, -5 deg C
	NTE stereoselective
RX(2)	RCT B 852392-86-0, E 77-76-9
	RGT G 24057-28-1 Pyridinium tosylate
	PRO F 852392-87-1
	CON 5 hours, room temperature
RX(3)	RCT F 852392-87-1, H 69739-34-0
	RGT J 108-48-5 2,6-Lutidine
	PRO I 852392-88-2
	SOL 75-09-2 CH2Cl2
	CON 15 minutes, 0 deg C
RX(4)	RCT I 852392-88-2
	RGT G 24057-28-1 Pyridinium tosylate
	PRO L 852392-89-3
	SOL 67-56-1 MeOH
	CON 2 hours, room temperature
RX(5)	RCT L 852392-89-3
	RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P 7758-89-6 CuCl
	PRO M 852392-90-6
	SOL 68-12-2 DMF
	CON 3 hours, room temperature
RX(6)	RCT M 852392-90-6, R 108-24-7
	RGT T 110-86-1 Pyridine, U 1122-58-3 4-DMAP
	PRO S 852392-91-7
	SOL 75-09-2 CH2Cl2
	CON 2.5 hours, 0 deg C

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L3 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 142:298056 CASREACT  
TITLE: Asymmetric Synthesis of (+)-(S,S)-Reboxetine via a New  
(S)-2-(Hydroxymethyl)morpholine Preparation  
AUTHOR(S): Brenner, Eric; Baldwin, Ronald M.; Tamagnan, Gilles  
CORPORATE SOURCE: Yale School of Medicine, VA Connecticut HCS, West  
Haven, CT, 06516, USA  
SOURCE: Organic Letters (2005), 7(5), 937-939  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Nonracemic (S,S)-reboxetine I (R = H) is prepared in eight steps and 30% overall yield; the key steps in the preparation of I are the selective oxidation of protected nonracemic hydroxymethylmorpholine II (R1 = Me3COCO; R2 = CH2OH) and nucleophilic aromatic substitution of the tricarbonylchromium complex of 1-ethoxy-2-fluorobenzene with nonracemic morpholinemethanol III. Chloroacetylation of (S)-3-amino-1,2-propanediol, regioselective cyclization mediated by potassium tert-butoxide in tert-amyl alc., reduction of the amide with Red-Al, and Boc protection of the morpholine nitrogen yields II (R1 = Me3COCO; R2 = CH2OH). Oxidation of II (R1 = Me3COCO; R2 = CH2OH) with TEMPO and trichloroisocyanuric acid in Et acetate with sodium bicarbonate yields II (R1 = Me3COCO; R2 = OHC) in 89% yield; oxidation of a substrate lacking the Boc protecting group or oxidation of II (R1 = Me3COCO; R2 = CH2OH) by Swern reaction gives either no reaction or epimerization, while the use of Et acetate decreases chlorination byproducts and the use of sodium bicarbonate neutralizes hydrogen chloride generated from the trichloroisocyanuric acid. Addition of II (R1 = Me3COCO; R2 = CHO) to diphenylzinc prepared from phenylmagnesium bromide and anhydrous zinc bromide

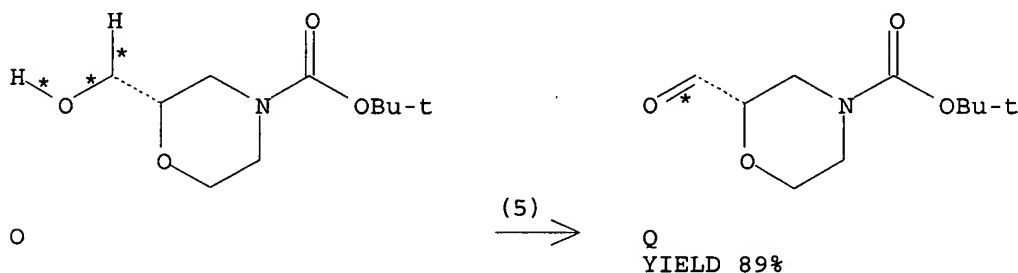
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in THF yields III in 60% yield in addition to 19% yield of the morpholinemethanol alc. epimer; the use of phenylmagnesium bromide as the nucleophile leads to aldehyde enolate formation and decreased yields of product. Nucleophilic aryl substitution of the tricarbonylchromium(0) complex of 1-ethoxy-2-fluorobenzene (prepared in two steps from 2-fluorophenol) with III and sodium hydride in DMF followed by oxidative demetalation with iodine in THF yields I (R = Me3COCO) in 95% yield; cleavage of the Boc group with TFA yields I (R = H). Mitsunobu reaction of the minor product of diphenylzinc addition to II (R1 = Me3COCO; R2 = OHC) with 2-ethoxyphenol followed by Boc cleavage also yields I (R = H); the yields of the Mitsunobu reaction do not exceed 53%.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 81 ...O ==> Q...



RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3  
SOL 141-78-6 AcOEt  
CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride  
SOL 141-78-6 AcOEt  
CON SUBSTAGE(1) 1 hour, -5 deg C  
SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)2  
SOL 7732-18-5 Water

PRO Q 847805-31-6

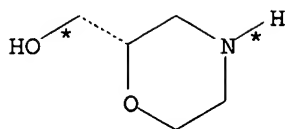
NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization, use of EtOAc suppresses chlorination

RX(15) OF 81 COMPOSED OF RX(4), RX(5)

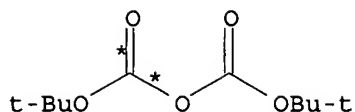
RX(15) K + N ==> Q

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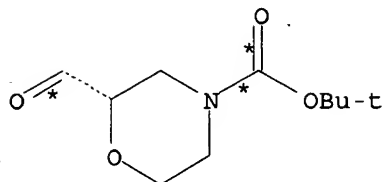


K



N

2  
STEPS  
→



Q  
YIELD 89%

RX(4) RCT K 132073-83-7, N 24424-99-5  
RGT P 1310-73-2 NaOH  
PRO O 135065-76-8  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 3 hours, room temperature

RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3  
SOL 141-78-6 AcOEt  
CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride  
SOL 141-78-6 AcOEt  
CON SUBSTAGE(1) 1 hour, -5 deg C  
SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)2  
SOL 7732-18-5 Water

PRO Q 847805-31-6

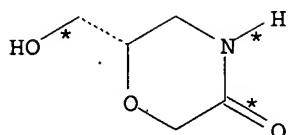
NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization,  
use of EtOAc suppresses chlorination

RX(26) OF 81 COMPOSED OF RX(3), RX(4), RX(5).

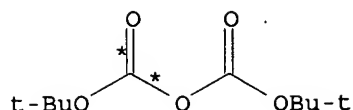
RX(26) G + N ==> Q

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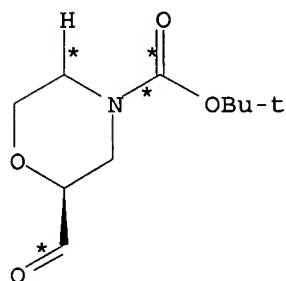


G



N

3  
STEPS  
→



Q  
YIELD 89%

RX(3) RCT G 847805-30-5

STAGE(1)

RGT L 22722-98-1 Red-Al

SOL 109-99-9 THF

CON SUBSTAGE(1) 1 hour, 0 deg C

SUBSTAGE(2) 16 hours, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RGT I 7732-18-5 Water

PRO K 132073-83-7

RX(4) RCT K 132073-83-7, N 24424-99-5

RGT P 1310-73-2 NaOH

PRO O 135065-76-8

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 3 hours, room temperature

RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3

SOL 141-78-6 AcOEt

CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) 1 hour, -5 deg C

SUBSTAGE(2) 1 hour, -5 deg C

Updated Search

## STAGE(3)

RGT U 3375-31-3 Pd(OAc)<sub>2</sub>

SOL 7732-18-5 Water

PRO Q 847805-31-6

NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization,  
use of EtOAc suppresses chlorination

L3 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:176596 CASREACT

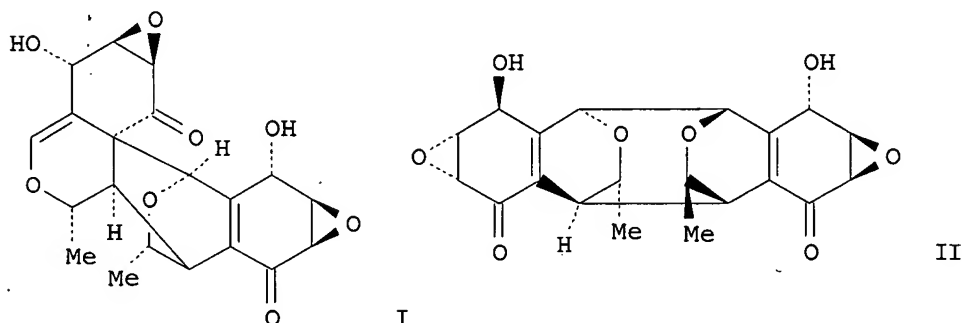
TITLE: Total Synthesis of Epoxyquinols A, B, and C and  
Epoxytwinol A and the Reactivity of a 2H-Pyran  
Derivative as the Diene Component in the Diels-Alder  
ReactionAUTHOR(S): Shoji, Mitsuru; Imai, Hiroki; Mukaida, Makoto; Sakai,  
Ken; Kakeya, Hideaki; Osada, Hiroyuki; Hayashi, YujiroCORPORATE SOURCE: Department of Industrial Chemistry, Faculty of  
Engineering, Department of Applied Chemistry, Faculty  
of Science, Tokyo University of Science, Shinjuku,  
Tokyo, 162-8601, JapanSOURCE: Journal of Organic Chemistry (2005), 70(1), 79-91  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



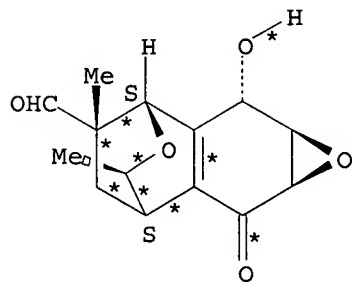
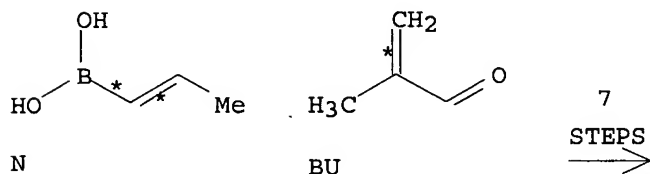
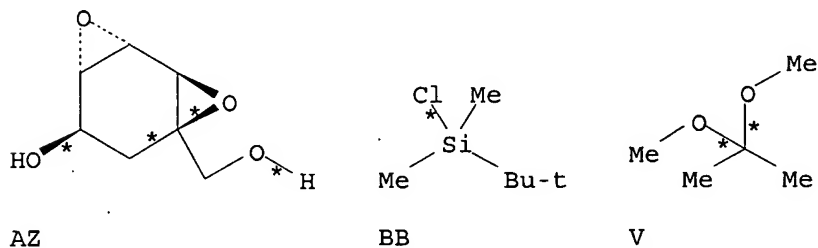
AB Full details of two versions of the total synthesis of epoxyquinols A, B, and C (I) and epoxytwinol A (II; RKB-3564D) are described. In the first-generation synthesis, the HfCl<sub>4</sub>-mediated diastereoselective Diels-Alder reaction of furan with Corey's chiral auxiliary has been developed. In the second-generation synthesis, a chromatog.-free preparation of an iodolactone, by using acryloyl chloride as the dienophile in the Diels-Alder reaction of furan, and the lipase-mediated kinetic resolution of a cyclohexenol derivative have been developed. This second-generation synthesis is suitable for large-scale preparation. A biomimetic cascade reaction involving oxidation, 6 $\pi$ -electrocyclization, and then Diels-Alder dimerization is the key reaction in the formation of the complex heptacyclic structure of epoxyquinols A, B, and C. Epoxytwinol A is synthesized by the cascade reaction composed of oxidation, 6 $\pi$ -electrocyclization, and formal [4+4] cycloaddn. reactions. A

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2H-pyran, generated by oxidation/6 $\pi$ -electrocyclization, acts as a good diene, reacting with several dienophiles to afford polycyclic compds. in one step. An azapentacyclic compound is synthesized by a similar cascade reaction composed of the four successive steps: oxidation, imine formation, 6 $\pi$ -azaelectrocyclization, and Diels-Alder dimerization.

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(111) OF 236 COMPOSED OF RX(13), RX(5), RX(4), RX(14), RX(3), RX(15), RX(23)  
 RX(111) AZ + BB + V + N + BU ==> BV



YIELD 69%

RX(13) RCT AZ 635678-63-6, BB 18162-48-6  
 RGT BC 121-44-8 Et3N, BD 1122-58-3 4-DMAP  
 PRO AA 488808-28-2  
 SOL 75-09-2 CH2Cl2  
 CON 15 hours, room temperature

RX(5) RCT AA 488808-28-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7758-02-3 KBr,

Updated Search



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AD 7681-52-9 NaOCl, AE 144-55-8 NaHCO<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water  
CON 40 minutes, -10 deg C, pH 9.5

STAGE(2)

RGT AF 7631-86-9 SiO<sub>2</sub>  
SOL 108-88-3 PhMe  
CON 4.5 hours, 70 deg C

PRO U 488808-29-3

RX(4) RCT U 488808-29-3

STAGE(1)

RGT X 9037-24-5 Amberlyst 15  
SOL 67-56-1 MeOH  
CON 5 hours, room temperature

STAGE(2)

RCT V 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 4 hours, room temperature

PRO W 488808-30-6

RX(14) RCT W 488808-30-6  
RGT AT 7553-56-2 I<sub>2</sub>, BE 2712-78-9 PhI(O<sub>2</sub>CCF<sub>3</sub>)<sub>2</sub>, BF 110-86-1 Pyridine  
PRO M 488808-31-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 22 hours, room temperature  
NTE in the dark

RX(3) RCT M 488808-31-7, N 7547-97-9

STAGE(1)

CAT 14220-64-5 PdCl<sub>2</sub>(PhCN)<sub>2</sub>, 20667-12-3 Ag<sub>2</sub>O, 603-32-7 Ph<sub>3</sub>As  
SOL 109-99-9 THF, 7732-18-5 Water  
CON 11 hours, room temperature

STAGE(2)

RGT P 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water  
CON 1 hour, room temperature

PRO O 238424-99-2  
NTE in the dark

RX(15) RCT O 238424-99-2  
RGT X 9037-24-5 Amberlyst 15  
PRO G 238424-94-7  
SOL 67-56-1 MeOH  
CON 40 minutes, room temperature

RX(23) RCT G 238424-94-7

STAGE(1)

RGT K 1313-13-9 MnO<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

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CON 1 hour, 0 deg C

STAGE(2)

RCT BU 78-85-3

CON room temperature

PRO BV 832731-77-8

NTE stereoselective

L3 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:424043 CASREACT

TITLE: Enantioselective total synthesis of epoxyquinone natural products (-)-phyllostine, (+)-epoxydon, (+)-epiepoxidon and (-)-panepophenanthrin: access to versatile chiral building blocks through enzymatic kinetic resolution

AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (2004), 45(41), 7683-7687

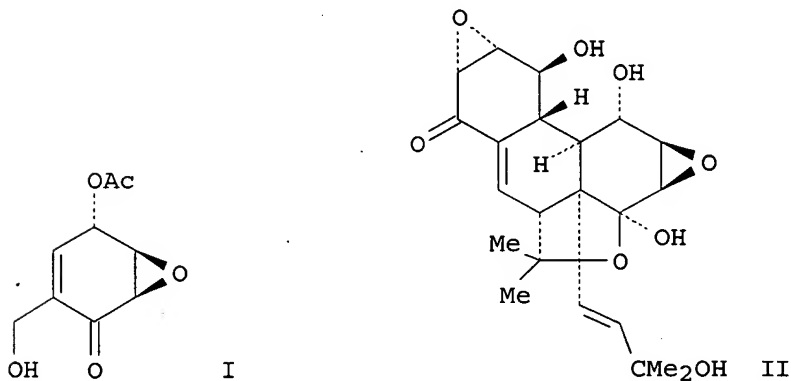
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



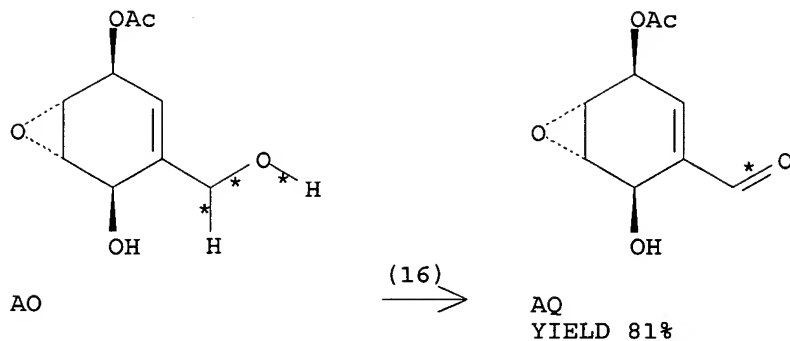
AB A new enzyme mediated protocol to access versatile chiral building blocks for the synthesis of epoxyquinone natural products is delineated. Total syntheses of (-)-phyllostine (I), (+)-epoxydon, (+)-epiepoxidon and (-)-panepophenanthrin (II) were accomplished to demonstrate the efficacy of this approach.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(16) OF 185 ...AO ==> AQ...

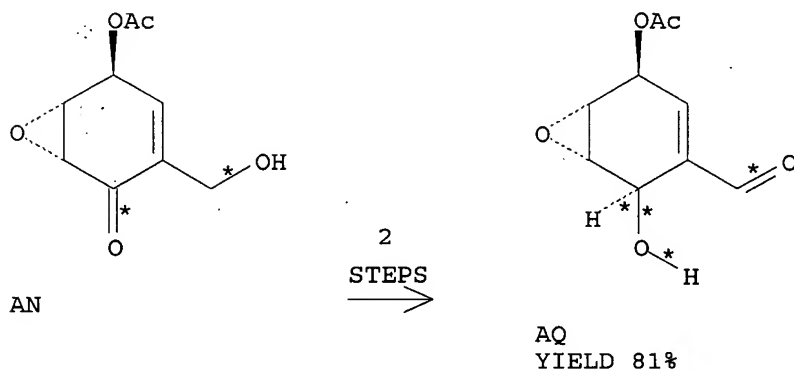
Updated Search

10509228



RX(16) RCT AO 792910-40-8  
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT 7782-44-7 O2  
PRO AQ 792910-42-0  
SOL 68-12-2 DMF  
CON room temperature

RX(36) OF 185 COMPOSED OF RX(15), RX(16)  
RX(36) AN ==> AQ



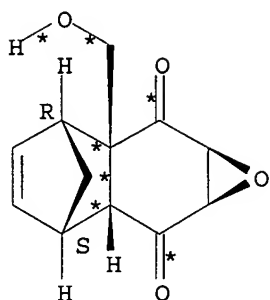
RX(15) RCT AN 792910-39-5  
RGT AP 1191-15-7 AlH(Bu-i)2  
PRO AO 792910-40-8  
SOL 109-99-9 THF  
CON -78 deg C

RX(16) RCT AO 792910-40-8  
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT 7782-44-7 O2  
PRO AQ 792910-42-0  
SOL 68-12-2 DMF  
CON room temperature

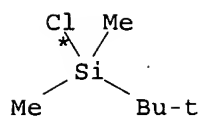
RX(116) OF 185 COMPOSED OF RX(6), RX(7), RX(8), RX(9), RX(14), RX(15), RX(16)  
RX(116) P + R + Z ==> AQ

Updated Search

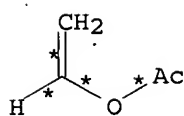
10509228



P

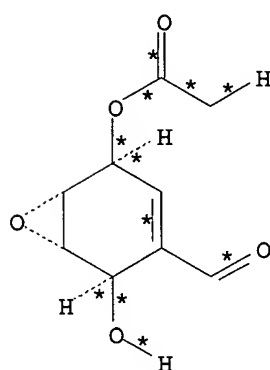


R



Z

7  
STEPS  
→



AQ

YIELD 81%

RX(6)	RCT	P 792910-31-7, R 18162-48-6
	RGT	T 288-32-4 1H-Imidazole
	PRO	S 792910-32-8
	CAT	1122-58-3 4-DMAP
	SOL	68-12-2 DMF
	CON	room temperature
RX(7)	RCT	S 792910-32-8
	RGT	X 16940-66-2 NaBH <sub>4</sub>
	PRO	W 792910-33-9
	SOL	67-56-1 MeOH
	CON	-15 deg C
RX(8)	RCT	W 792910-33-9, Z 108-05-4
	PRO	AA 792910-49-7, AB 792910-34-0
	CAT	9001-62-1 Lipase
	SOL	108-05-4 Vinyl acetate
	CON	room temperature
	NTE	enzymic
RX(9)	RCT	AB 792910-34-0
	PRO	AD 792910-35-1
	SOL	101-84-8 PhOPh

Updated Search

10509228

CON 5 minutes, 240 deg C

RX(14) RCT AD 792910-35-1  
RGT C 62778-11-4 Olah's reagent  
PRO AN 792910-39-5  
SOL 109-99-9 THF  
CON 0 deg C

RX(15) RCT AN 792910-39-5  
RGT AP 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO AO 792910-40-8  
SOL 109-99-9 THF  
CON -78 deg C

RX(16) RCT AO 792910-40-8  
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT  
7782-44-7 O<sub>2</sub>  
PRO AQ 792910-42-0  
SOL 68-12-2 DMF  
CON room temperature

L3 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:410727 CASREACT

TITLE: Total Synthesis of the Novel, Biologically Active  
Epoxyquinone Dimer (±)-Torreyanic Acid: A  
Biomimetic Approach

AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of  
Science, Bangalore, 560 012, India

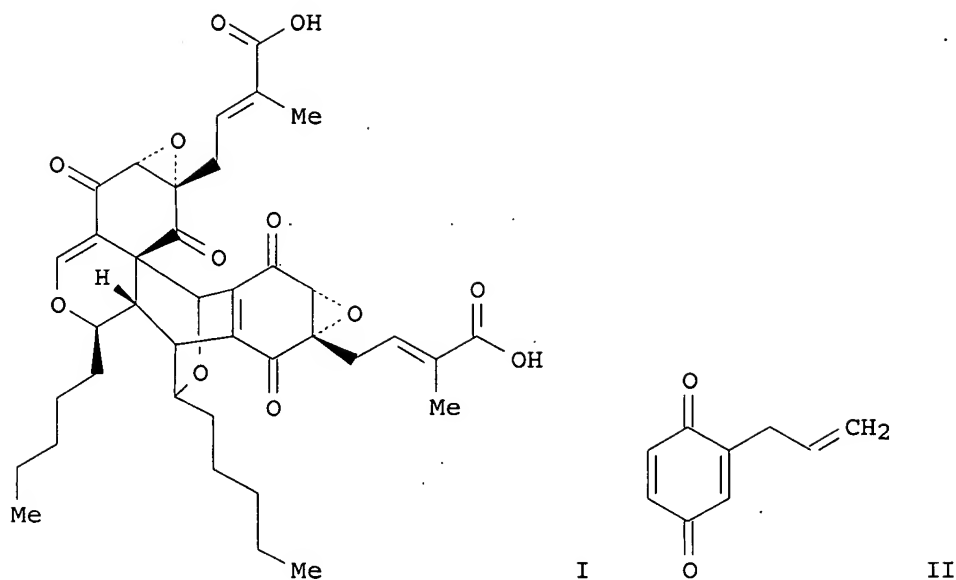
SOURCE: Organic Letters (2004), 6(22), 3985-3988  
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

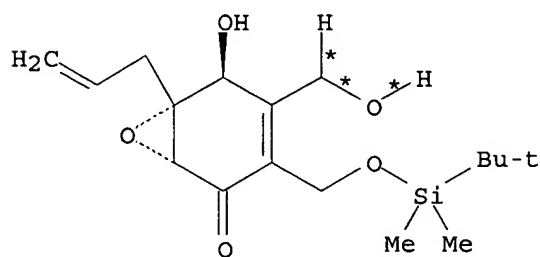
GI



AB A total synthesis of the complex, biol. active, dimeric natural product ( $\pm$ )-torreyanic acid (I), which is composed of seven rings and laced with dense oxy-functionalization, has been accomplished from readily available allyl-substituted p-benzoquinone II. Our synthetic stratagem involves crafting an epoxyquinone monomer for use in a biomimetic cascade process involving a tandem  $6\pi$  electrocyclization and a Diels-Alder dimerization.

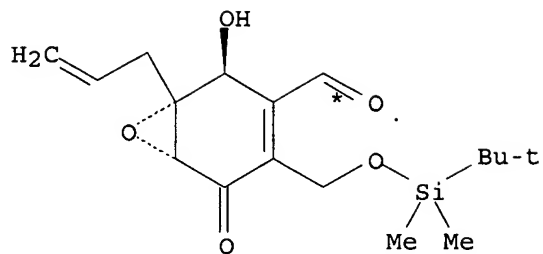
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 230 ...Y ==> AA...



(9)  $\longrightarrow$

10509228



AA

YIELD 90%

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

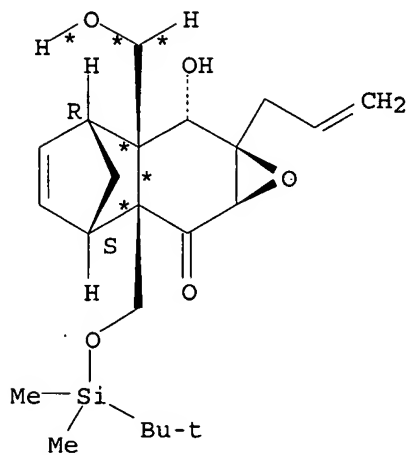
SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(29) OF 230 COMPOSED OF RX(8), RX(9)

RX(29) W ==> AA

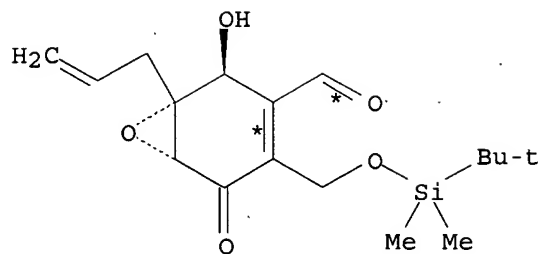


W

2  
STEPS  
→

Updated Search

10509228



AA

YIELD 90%

RX(8) RCT W 791854-38-1  
RGT Z 101-84-8 PhOPh  
PRO Y 791854-39-2  
CON 6 minutes, 220 deg C  
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

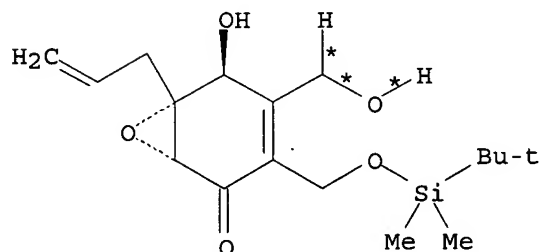
STAGE(2)

RGT AD 7758-98-7 CuSO4  
SOL 7732-18-5 Water

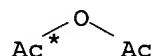
PRO AA 791854-32-5  
NTE chemoselective

RX(30) OF 230 COMPOSED OF RX(9), RX(10)

RX(30) Y + AE ==> AF



Y



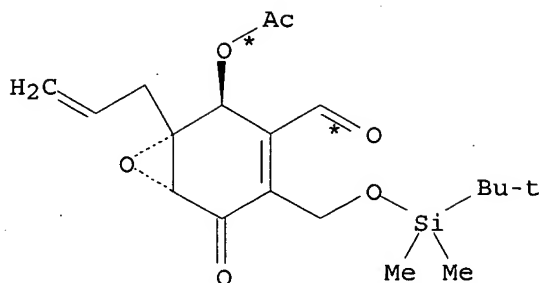
AE

2  
STEPS  
→

Updated Search



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AF  
YIELD 98%

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

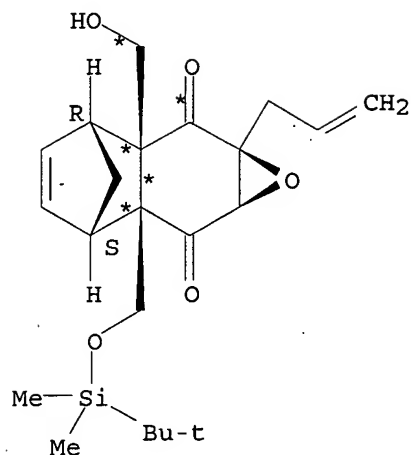
RGT D 7732-18-5 Water

PRO AF 791854-40-5

RX(53) OF 230 COMPOSED OF RX(7), RX(8), RX(9)

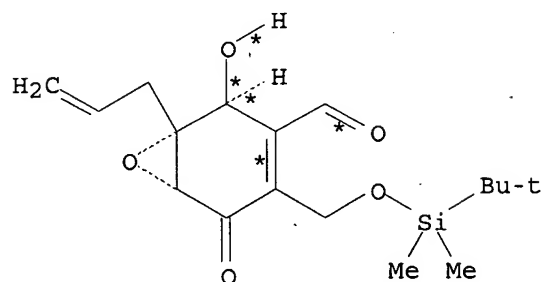
RX(53) V ==> AA

10509228



V

3  
STEPS  
→



AA

YIELD 90%

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH<sub>4</sub>

SOL 67-56-1 MeOH

CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1

NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

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STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

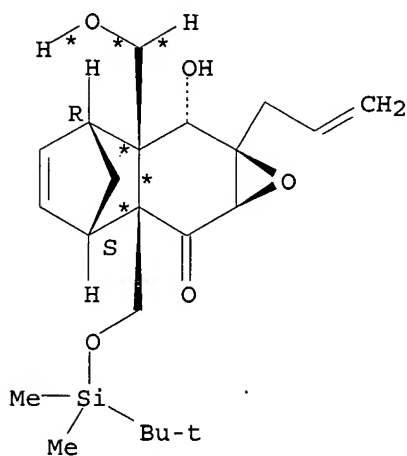
SOL 7732-18-5 Water

PRO AA 791854-32-5

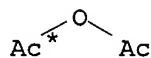
NTE chemoselective

RX(55) OF 230 COMPOSED OF RX(8), RX(9), RX(10)

RX(55) W + AE ==> AF

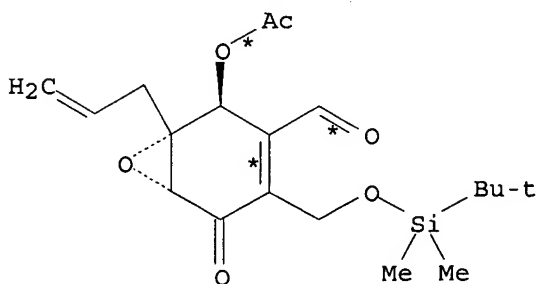


W



AE

3  
STEPS  
→



AF

YIELD 98%

RX(8)

RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

Updated Search

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NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

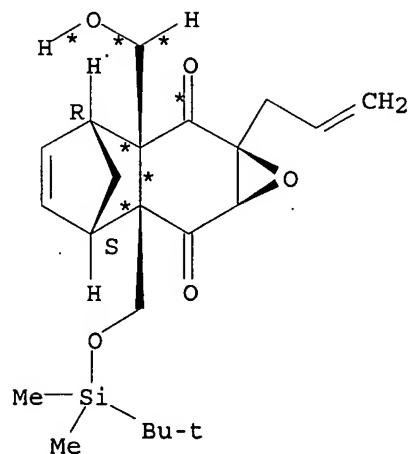
STAGE(2)

RGT D 7732-18-5 Water

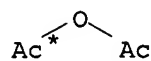
PRO AF 791854-40-5

RX(56) OF 230 COMPOSED OF RX(7), RX(8), RX(9), RX(10)

RX(56) V + AE ==> AF



V

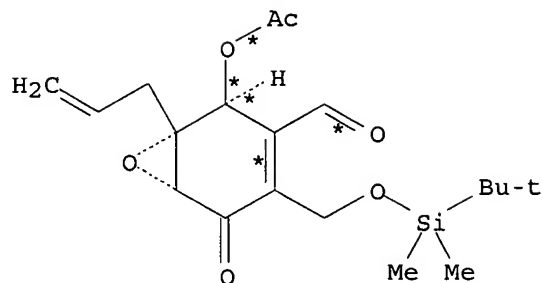


AE

4  
STEPS  
→

Updated Search

10509228



AF  
YIELD 98%

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH<sub>4</sub>

SOL 67-56-1 MeOH

CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1

NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me<sub>4</sub>-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO<sub>4</sub>

SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

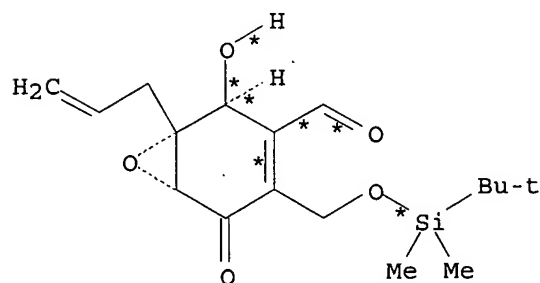
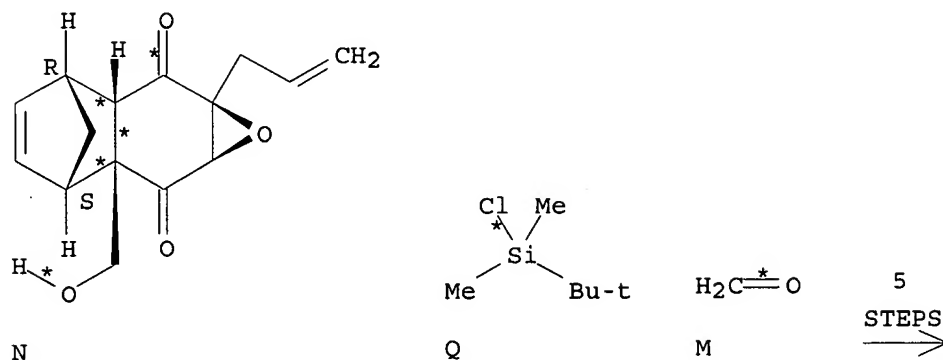
RGT D 7732-18-5 Water

Updated Search

10509228

PRO AF 791854-40-5

RX(89) OF 230 COMPOSED OF RX(5), RX(6), RX(7), RX(8), RX(9)  
RX(89) N + Q + M ==> AA



AA  
YIELD 90%

RX(5) RCT N 791854-36-9, Q 18162-48-6

STAGE(1)

RGT S 288-32-4 1H-Imidazole  
CAT 1122-58-3 4-DMAP  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water  
CON room temperature

PRO R 791854-37-0

RX(6) RCT R 791854-37-0

STAGE(1)

RGT O 6674-22-2 DBU

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10509228

SOL 109-99-9 THF  
CON 1 hour, 0 deg C

STAGE(2)

RCT M 50-00-0  
SOL 7732-18-5 Water  
CON 36 hours, room temperature

PRO V 791854-33-6  
NTE stereoselective

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH4  
SOL 67-56-1 MeOH  
CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1  
NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1  
RGT Z 101-84-8 PhOPh  
PRO Y 791854-39-2  
CON 6 minutes, 220 deg C  
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

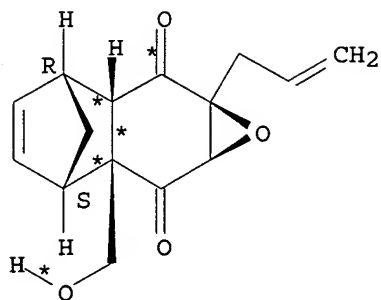
STAGE(2)

RGT AD 7758-98-7 CuSO4  
SOL 7732-18-5 Water

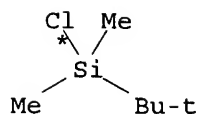
PRO AA 791854-32-5  
NTE chemoselective

RX(94) OF 230 COMPOSED OF RX(5), RX(6), RX(7), RX(8), RX(9), RX(10)  
RX(94) N + Q + M + AE ==> AF

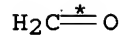
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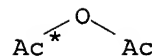
N



Q

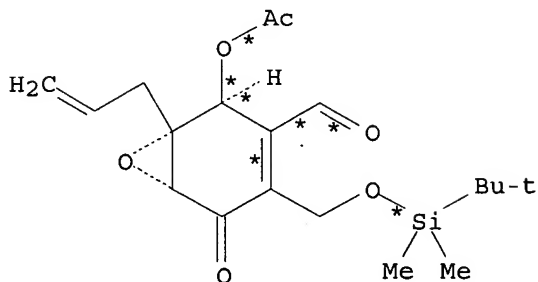


M



AE

6  
STEPS  
→



AF

YIELD 98%

RX(5) RCT N 791854-36-9, Q 18162-48-6

STAGE(1)

RGT S 288-32-4 1H-Imidazole

CAT 1122-58-3 4-DMAP

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water

CON room temperature

PRO R 791854-37-0

RX(6) RCT R 791854-37-0

STAGE(1)

RGT O 6674-22-2 DBU

SOL 109-99-9 THF

CON 1 hour, 0 deg C

Updated Search



10509228

STAGE(2)

RCT M 50-00-0  
SOL 7732-18-5 Water  
CON 36 hours, room temperature

PRO V 791854-33-6  
NTE stereoselective

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH4  
SOL 67-56-1 MeOH  
CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1  
NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1  
RGT Z 101-84-8 PhOPh  
PRO Y 791854-39-2  
CON 6 minutes, 220 deg C  
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4  
SOL 7732-18-5 Water

PRO AA 791854-32-5  
NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water

PRO AF 791854-40-5

L3 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:410671 CASREACT

TITLE: The oxidation of alcohols in N-Oxyl-immobilized silica

Updated Search

10509228

gel/aqueous NaOCl disperse systems. A prominent access to a column-flow system

AUTHOR(S): Tanaka, Hideo; Chou, Jingyu; Mine, Machiko; Kuroboshi, Manabu

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Okayama University, Okayama, 700-8530, Japan

SOURCE: Bulletin of the Chemical Society of Japan (2004), 77(9), 1745-1755  
CODEN: BCSJA8; ISSN: 0009-2673

PUBLISHER: Chemical Society of Japan

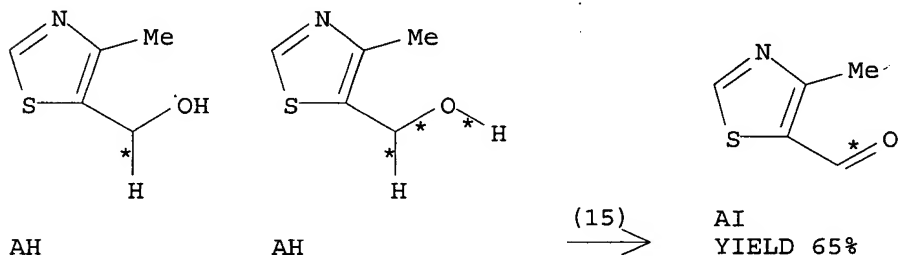
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The oxidation of alcs. was performed successfully in a disperse system with N-oxyl-adsorbed or immobilized silica gel as a disperse phase and aqueous NaOCl as a disperse medium. In the disperse system, the oxidation of sec-alcs. afforded the corresponding ketones, while prim-alcs. were oxidized to aldehydes and/or carboxylic acids depending on their structures and reaction conditions. The N-oxyl-immobilized silica gel was recovered and repeatedly used without a significant change in the product yields. A column-flow system was also investigated for the oxidation of alcs. by use of a newly devised column packed with the N-oxyl-immobilized silica gel.

REFERENCE COUNT: 142 THERE ARE 142 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

RX(15) OF 33 2 AH ==> AI + AJ



AJ  
YIELD 11%

RX(15) RCT AH 1977-06-6

STAGE(1)

RGT C 3225-26-1 Piperidinoxy deriv., D 7631-86-9

Updated Search

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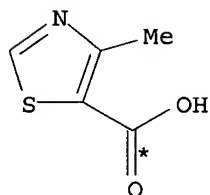
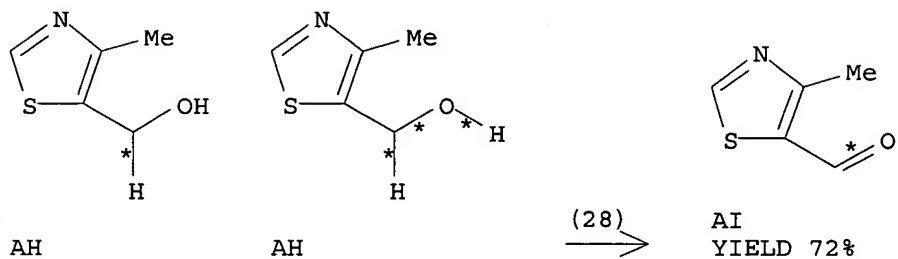
SiO2  
SOL 67-64-1 Me2CO  
CON 10 minutes, room temperature

STAGE(2)

RGT E 7681-52-9 NaOCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 2 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

RX(28) OF 33 2 AH ==> AI + AJ



AJ  
YIELD 15%

RX(28) RCT AH 1977-06-6

STAGE(1)

RGT AU 21216-79-5D 1-Piperidinyloxy,  
4-[(aminocarbonyl)amino]-2,2,6,6-tetramethyl-  
SOL 67-64-1 Me2CO  
CON 10 minutes, room temperature

STAGE(2)

RGT E 7681-52-9 NaOCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 0.5 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

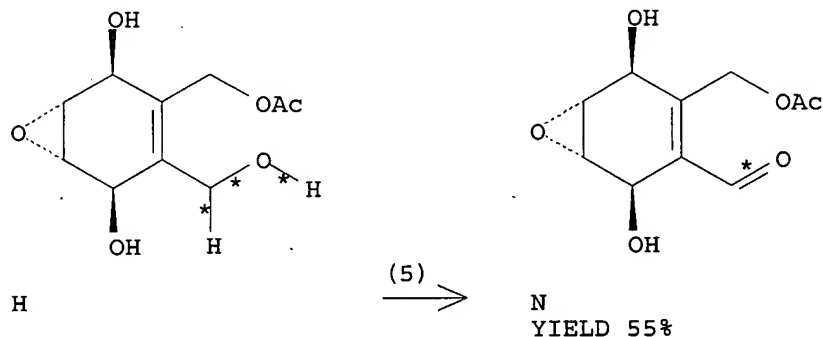
L3 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

ACCESSION NUMBER: 141:206943 CASREACT  
TITLE: Enantioselective Total Synthesis of (+)-Eupenoxide and (+)-Phomoxide: Revision of Structures and Assignment of Absolute Configuration  
AUTHOR(S): Mehta, Goverdhan; Roy, Subhrangsu  
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India  
SOURCE: Organic Letters (2004), 6(14), 2389-2392  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Stereo- and enantioselective total syntheses of the novel, polyketide natural products ent-eupenoxide and ent-phomoxide were accomplished from the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone. These synthetic studies necessitate the revision of the assigned stereostructures of the natural products and reveal their absolute configuration.  
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

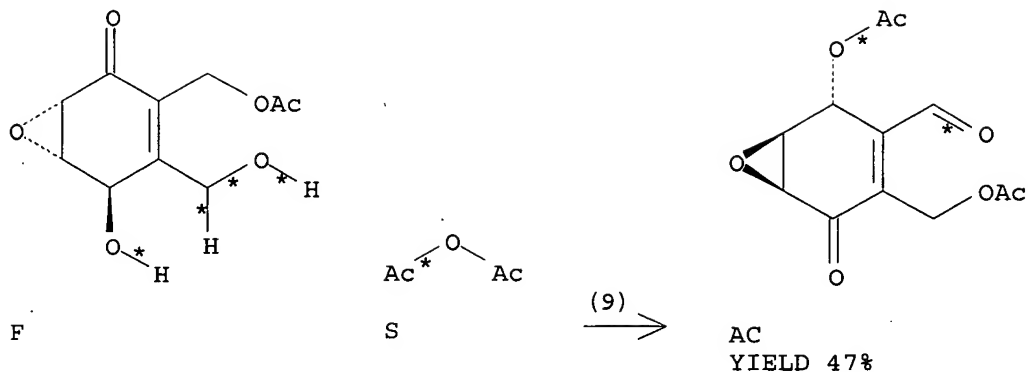
RX(5) OF 87 ...H ==> N...



RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(9) OF 87 ...F + S ==> AC...

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RX(9) RCT F 676263-76-6

STAGE(1)

RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl

SOL 68-12-2 DMF

STAGE(2)

RCT S 108-24-7

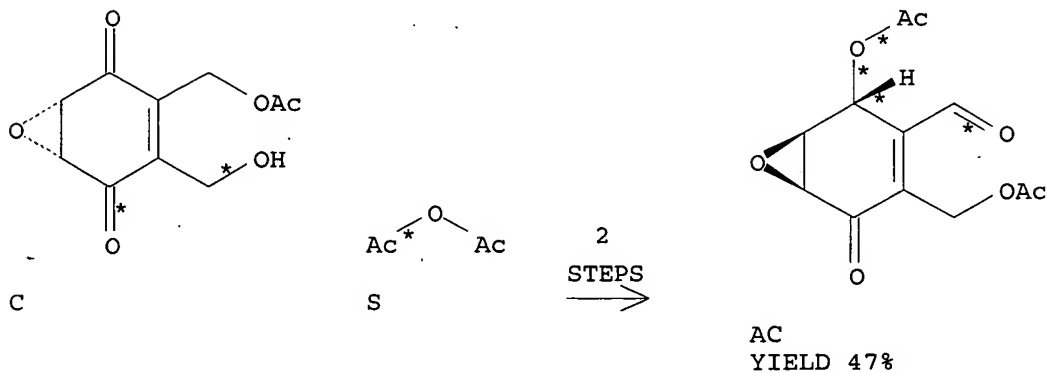
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

PRO AC 676263-80-2

RX(21) OF 87 COMPOSED OF RX(2), RX(9)

RX(21) C + S ==> AC



RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)2  
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(9) RCT F 676263-76-6

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STAGE(1)

RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
SOL 68-12-2 DMF

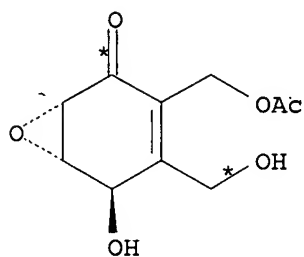
STAGE(2)

RCT S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2

PRO AC 676263-80-2

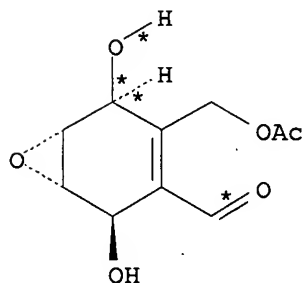
RX(23) OF 87 COMPOSED OF RX(3), RX(5)

RX(23) F ==> N



F

2  
STEPS  
→



N

YIELD 55%

RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3  
PRO H 735317-25-6  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

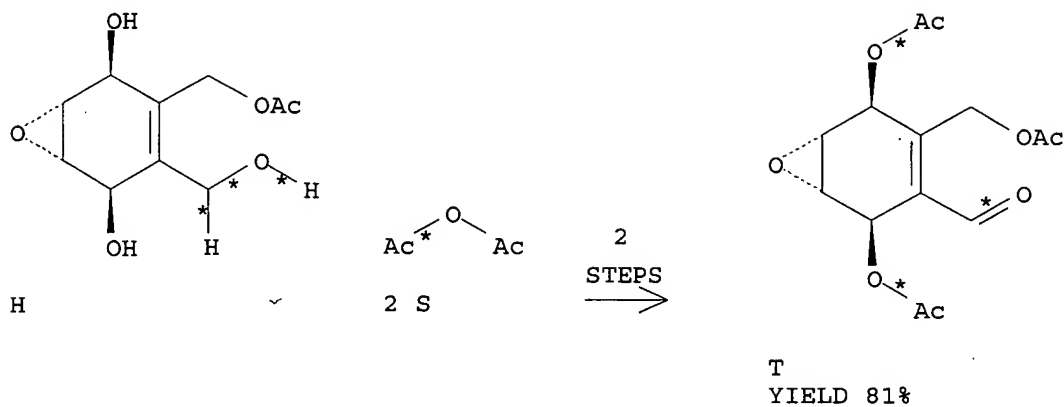
RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

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RX(24) OF 87 COMPOSED OF RX(5), RX(6)

RX(24) H + 2 S ==> T

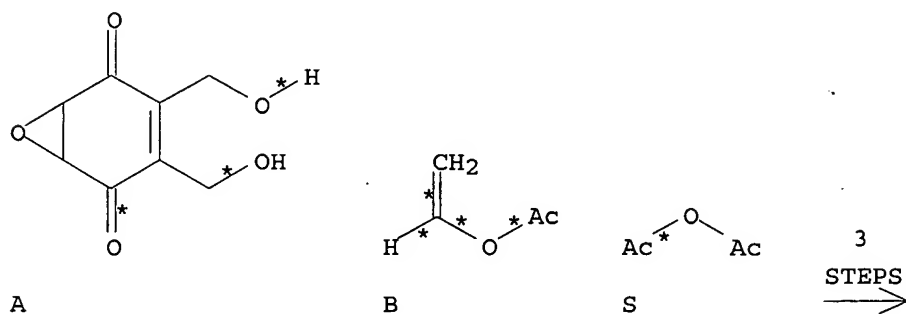


RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

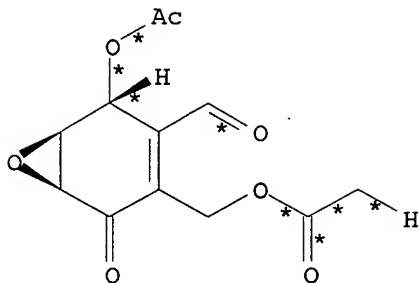
RX(6) RCT N 735317-27-8, S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
PRO T 735317-28-9  
SOL 75-09-2 CH2Cl2

RX(37) OF 87 COMPOSED OF RX(1), RX(2), RX(9)

RX(37) A + B + S ==> AC



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AC  
YIELD 47%

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 109-99-9 THF  
CON 0 deg C  
NTE biotransformation, enzymic(lipase PS)

RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)2  
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(9) RCT F 676263-76-6

STAGE(1)

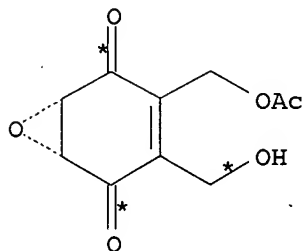
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
SOL 68-12-2 DMF

STAGE(2)

RCT S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2

PRO AC 676263-80-2

RX(39) OF 87 COMPOSED OF RX(2), RX(3), RX(5)  
RX(39) C ==> N



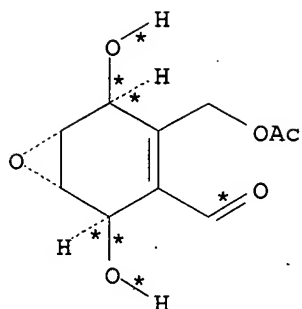
C

3  
STEPS  
→

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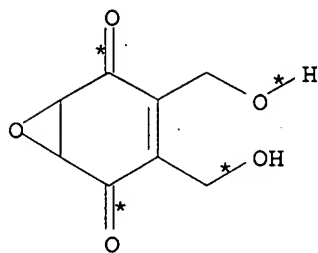
N  
YIELD 55%

RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

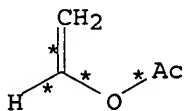
RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH<sub>4</sub>, J 7790-86-5 CeCl<sub>3</sub>  
PRO H 735317-25-6  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me<sub>4</sub>-piperidoxyl, P 7782-44-7 O<sub>2</sub>, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(43) OF 87 COMPOSED OF RX(1), RX(2), RX(3), RX(5)  
RX(43) A + B ==> N



A

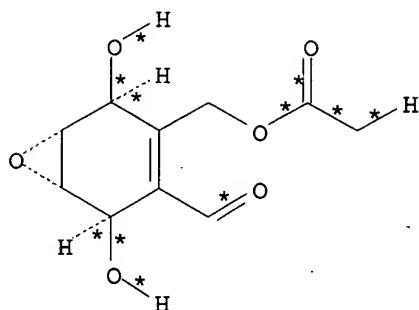


B

4  
STEPS  
→

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N  
YIELD 55%

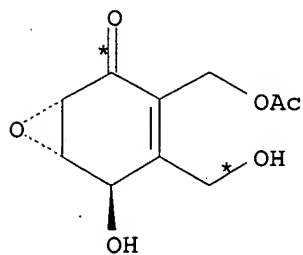
RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 109-99-9 THF  
CON 0 deg C  
NTE biotransformation, enzymic(lipase PS)

RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)2  
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

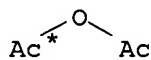
RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3  
PRO H 735317-25-6  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(46) OF 87 COMPOSED OF RX(3), RX(5), RX(6)  
RX(46) F + 2 S ==> T



F

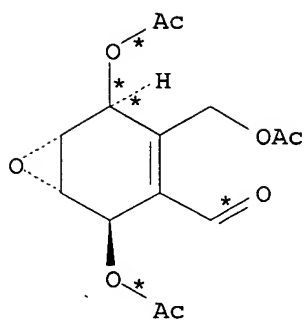


2 S

3  
STEPS  
→

Updated Search

10509228



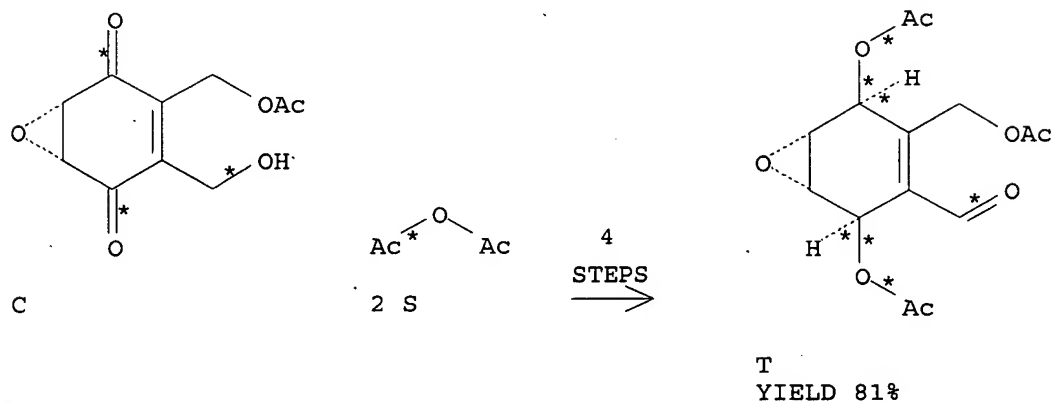
T  
YIELD 81%

RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH<sub>4</sub>, J 7790-86-5 CeCl<sub>3</sub>  
PRO H 735317-25-6  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me<sub>4</sub>-piperidoxyl, P 7782-44-7 O<sub>2</sub>, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
PRO T 735317-28-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(47) OF 87 COMPOSED OF RX(2), RX(3), RX(5), RX(6)  
RX(47) C + 2 S ==> T



RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)<sub>2</sub>

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10509228

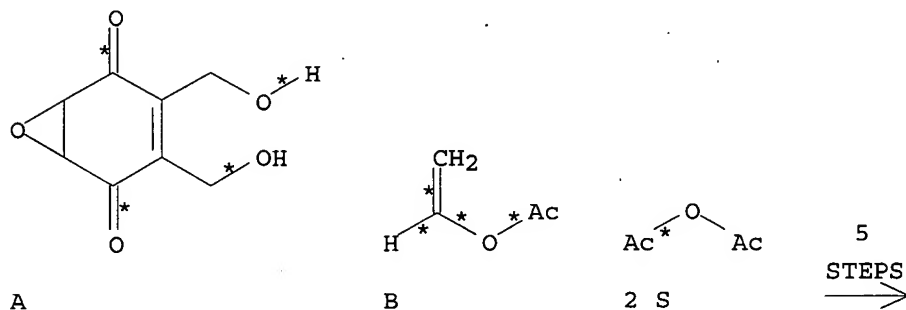
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH<sub>4</sub>, J 7790-86-5 CeCl<sub>3</sub>  
PRO H 735317-25-6  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me<sub>4</sub>-piperidoxyl, P 7782-44-7 O<sub>2</sub>, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
PRO T 735317-28-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(66) OF 87 COMPOSED OF RX(1), RX(2), RX(3), RX(5), RX(6)  
RX(66) A + B + 2 S ==> T



T  
YIELD 81%

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RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 109-99-9 THF  
CON 0 deg C  
NTE biotransformation, enzymic(lipase PS)

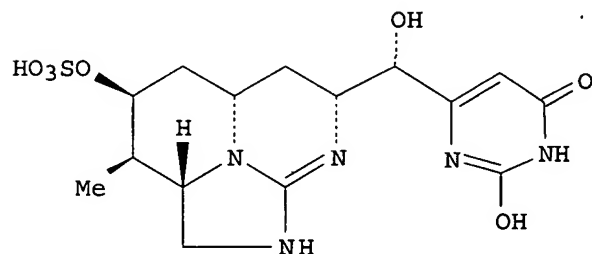
RX(2) RCT C 676263-74-4  
RGT G 1191-15-7 AlH(Bu-i)2  
PRO F 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(3) RCT F 676263-76-6  
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3  
PRO H 735317-25-6  
SOL 67-56-1.MeOH  
CON 0 deg C  
NTE stereoselective

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7  
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP  
PRO T 735317-28-9  
SOL 75-09-2 CH2Cl2

L3 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 141:174352 CASREACT  
TITLE: A concise asymmetric synthesis of the marine  
hepatotoxin 7-epicyclindrospermopsin  
AUTHOR(S): Looper, Ryan E.; Williams, Robert M.  
CORPORATE SOURCE: Department of Chemistry, Colorado State University,  
Fort Collins, CO, 80523, USA  
SOURCE: Angewandte Chemie, International Edition (2004),  
43(22), 2930-2933  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

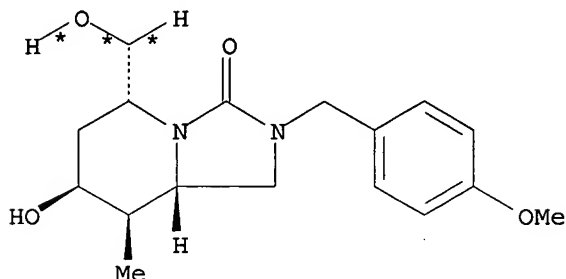
Updated Search

10509228

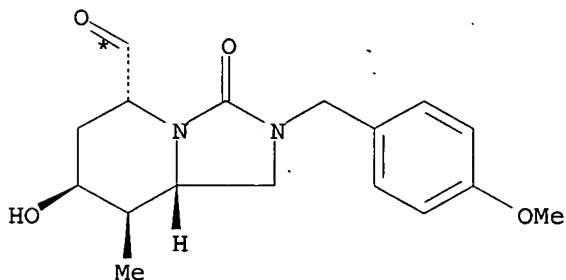
AB Born from a simple amino acid, the potent hepatotoxic cyanobacterial alkaloid 7-epicyclindropermopsin (I) was synthesized through a concise asym. eighteen-step route. An intramol. 1,3-dipolar cycloaddn. and a nitroaldol reaction are key steps in the construction of the natural product from a precursor with a single stereogenic center.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 120 ...V ==> H...



V



H

YIELD 75%

RX(6) RCT V 732278-69-2  
RGT W 3240-34-4 PhI(OAc)<sub>2</sub>, X 2564-83-2 Me<sub>4</sub>-piperidoxyl, Y  
75-75-2 MeSO<sub>3</sub>H  
PRO H 732278-68-1  
SOL 865-49-6 CDCl<sub>3</sub>  
CON 3 hours, room temperature

L3 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:54113 CASREACT

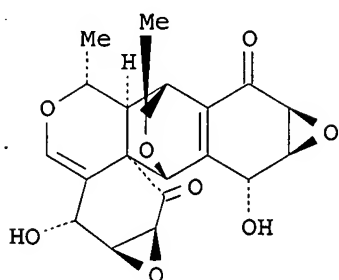
TITLE: Enantioselective total synthesis of (-)-epoxyquinols A and B. Novel, convenient access to chiral epoxyquinone building blocks through enzymatic desymmetrization

AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul

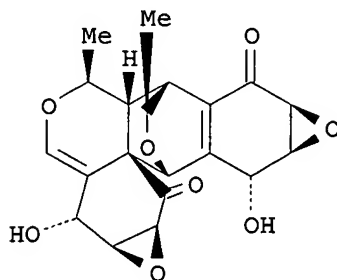
Updated Search

10509228

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India  
SOURCE: Tetrahedron Letters (2004), 45(18), 3611-3615  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

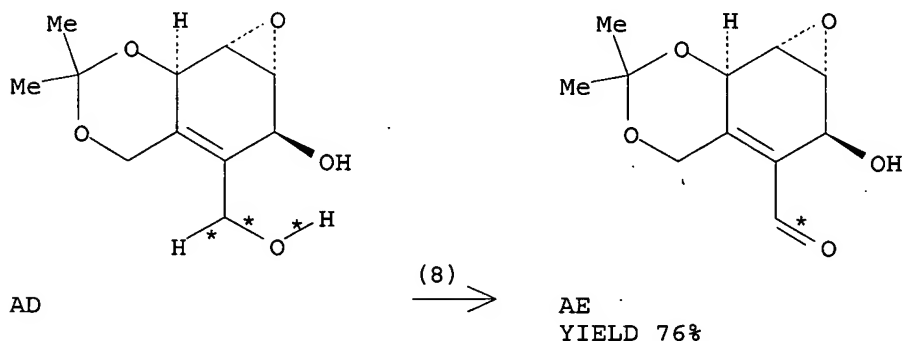


II

AB Following our recent total synthesis of the biol. potent natural products epoxyquinols A and B in racemic form, we have now accomplished the total synthesis of the (-)-epoxyquinols A (I) and B (II), antipodes of the angiogenesis inhibiting natural products, through a protocol that involves enzymic desymmetrization of a versatile epoxyquinone derivative, readily available from the Diels-Alder adduct of cyclopentadiene and p-benzoquinone.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(8) OF 307 ...AD ==> AE...

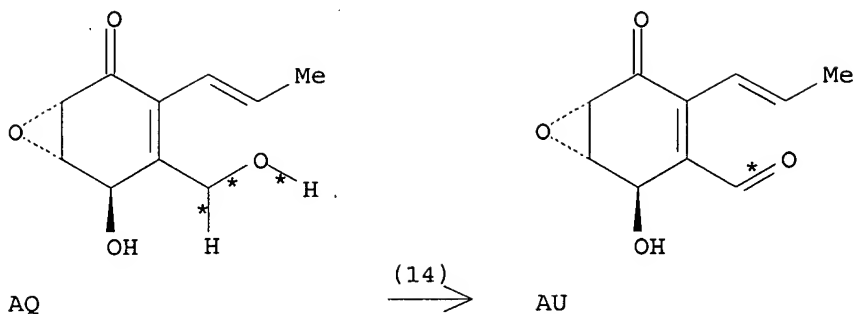


RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(14) OF 307 ...AQ ==> AU...

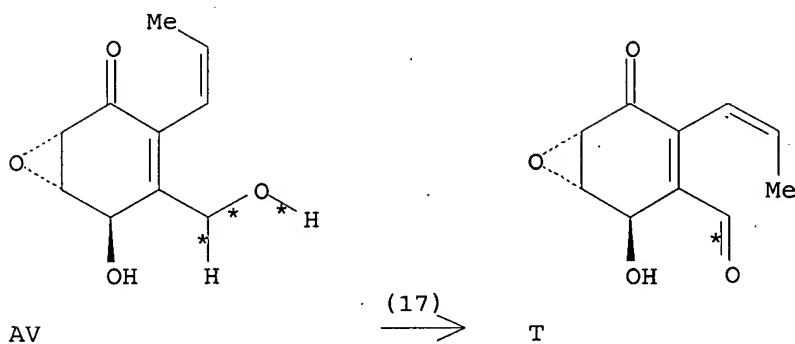
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RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(17) OF 307 ...AV ==> T...



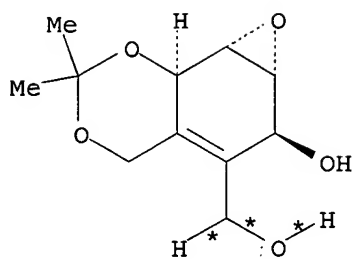
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(31) OF 307 COMPOSED OF RX(8), RX(9)  
RX(31) AD + O ==> AJ

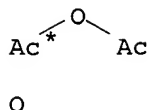
Updated Search



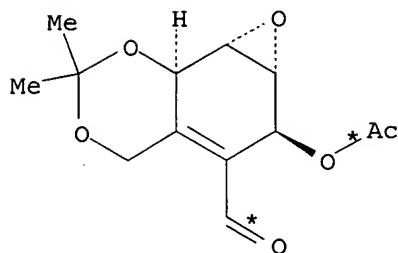
10509228



AD



2  
STEPS  
→



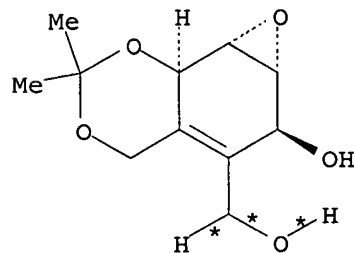
AJ

YIELD 87%

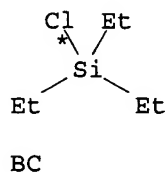
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

RX(32) OF 307 COMPOSED OF RX(8), RX(22)  
RX(32) AD + BC ==> BD



AD

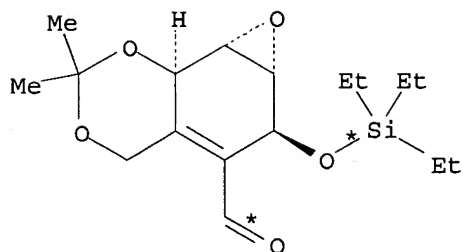


BC

2  
STEPS  
→

Updated Search

10509228

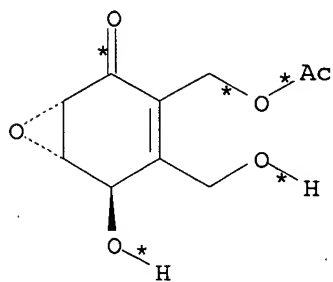


BD  
YIELD 70%

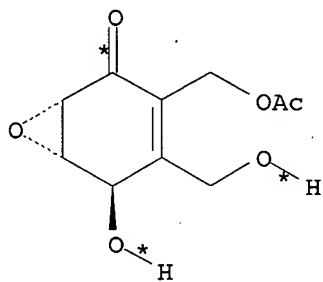
RX(8)      RCT    AD 701921-79-1  
             RGT    AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
                  Me4-piperidoxyl  
             PRO    AE 701921-80-4  
             SOL    68-12-2 DMF

RX(22)    RCT    AE 701921-80-4, BC 994-30-9  
             RGT    BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
             PRO    BD 701921-90-6  
             SOL    75-09-2 CH2Cl2  
             CON    0 deg C

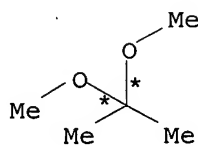
RX(57) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8)  
 RX(57)    2 L + 2 W ==> AE



L



L

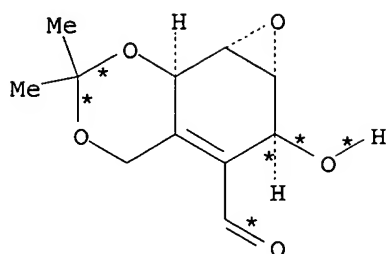


2 W

4  
STEPS  
→

Updated Search

10509228



AE

YIELD 76%

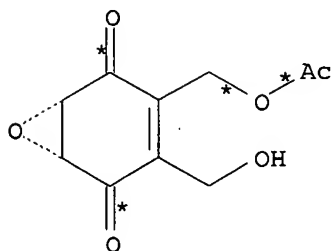
RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

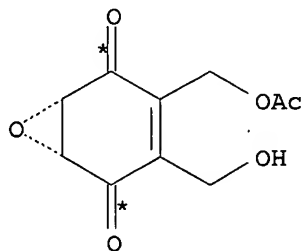
RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

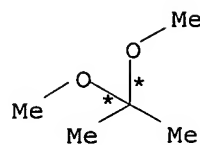
RX(109) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8)  
RX(109) 2 C + 2 W ==> AE



C



C

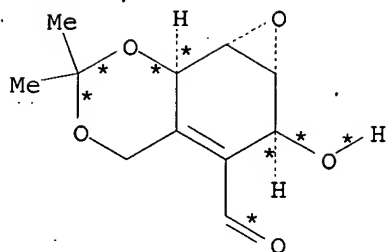


2 W

Updated Search

10509228

5  
STEPS  
→



AE  
YIELD 76%

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)2  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

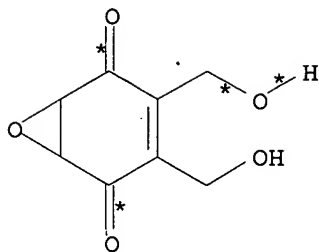
RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

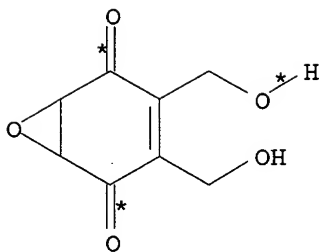
RX(110) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8)  
RX(110) 2 A + 2 B + 2 W ==> AE

Updated Search

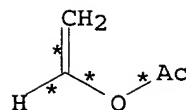
10509228



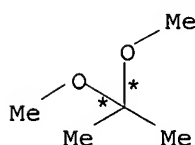
A



A

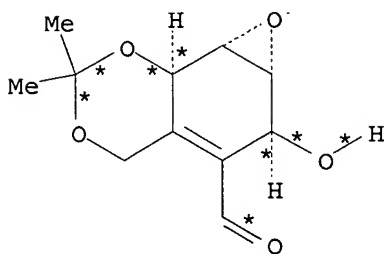


2 B



2 W

6  
STEPS  
→



AE

YIELD 76%

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

Updated Search

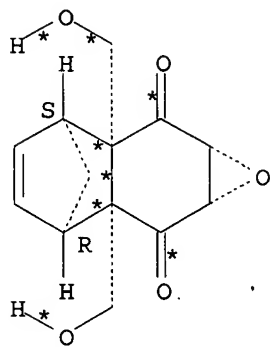
10509228

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

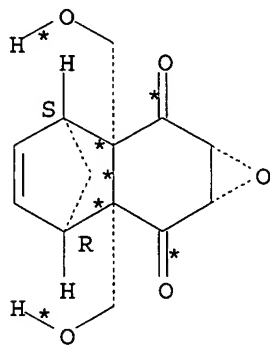
RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

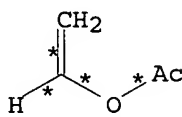
RX(111) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8)  
RX(111) 2 AX + 2 B + 2 W ==> AE



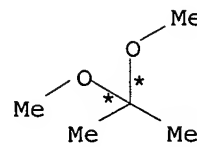
AX



AX



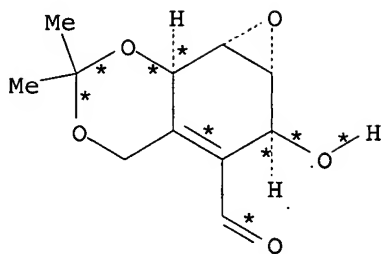
2 B



2 W

7  
STEPS  
→

10509228



AE

YIELD 76%

RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

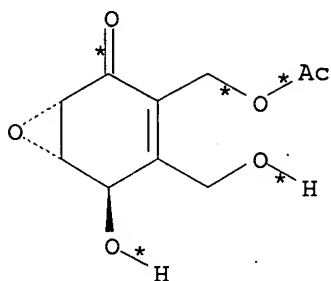
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl

Updated Search

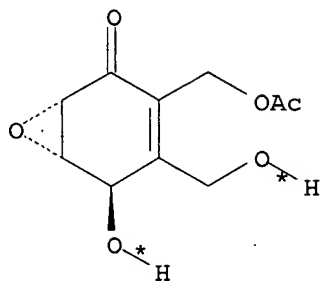
10509228

PRO AE 701921-80-4  
SOL 68-12-2 DMF

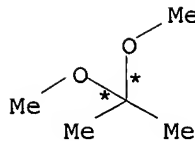
RX(113) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9)  
RX(113) 2 L + 2 W + O ==> AJ



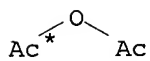
L



L

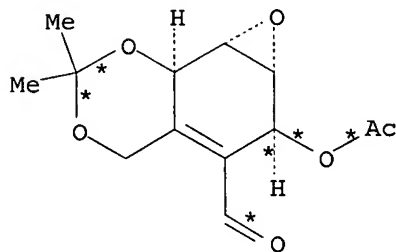


2 W



O

5  
STEPS  
→



AJ  
YIELD 87%

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3

Updated Search



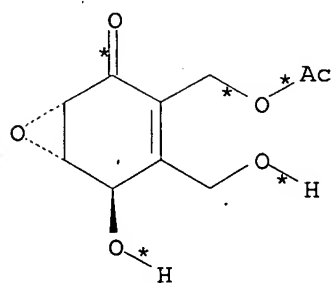
10509228

RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

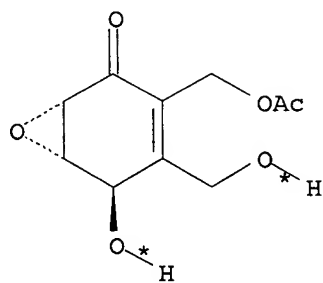
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

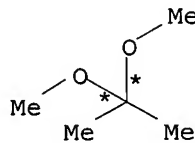
RX(114) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22)  
RX(114) 2 L + 2 W + BC ==> BD



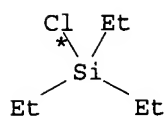
L



L

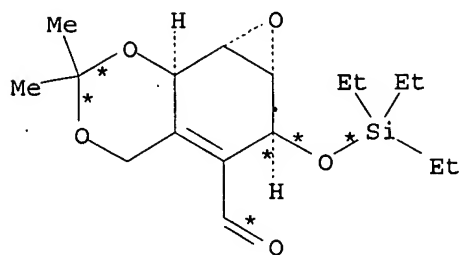


2 W



BC

5  
STEPS  
→



BD  
YIELD 70%

Updated Search

10509228

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

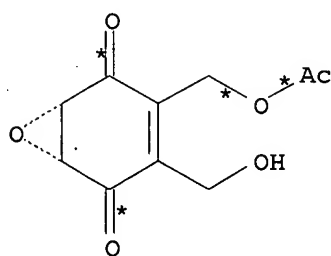
RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

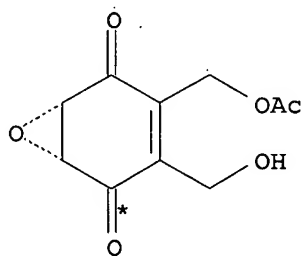
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

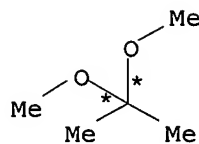
RX(115) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9)  
RX(115) 2 C + 2 W + O ==> AJ



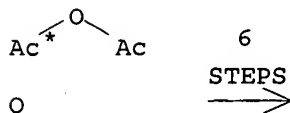
C



C



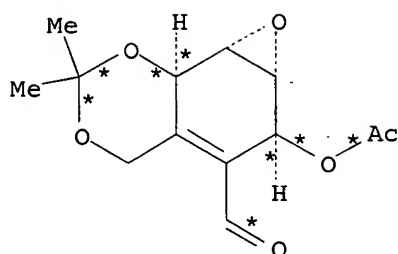
2 W



6  
STEPS  
→

Updated Search

10509228



AJ

YIELD 87%

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

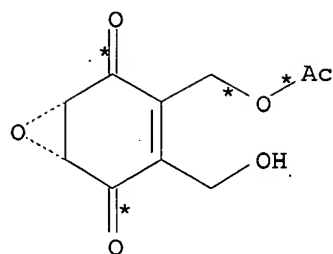
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

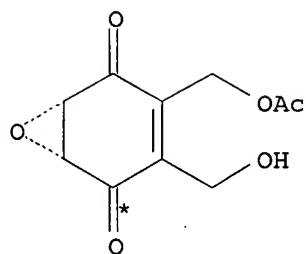
RX(116) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22)  
RX(116) 2 C + 2 W + BC ==> BD

Updated Search

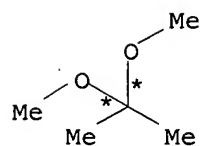
10509228



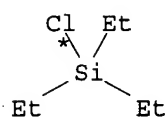
C



C

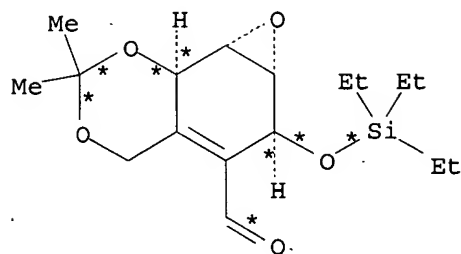


2 W



BC

6  
STEPS  
→



BD

YIELD 70%

RX(3)	RCT	C 676263-74-4
	RGT	M 1191-15-7 AlH(Bu-i) <sub>2</sub>
	PRO	L 676263-76-6
	SOL	109-99-9 THF
	CON	-78 deg C
	NTE	stereoselective
RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me <sub>2</sub> CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH <sub>4</sub>
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl <sub>3</sub>
	SOL	67-56-1 MeOH
	CON	0 deg C

Updated Search

10509228

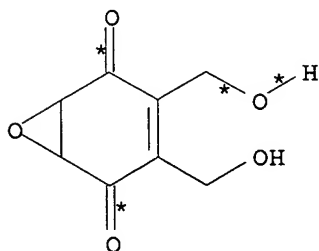
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

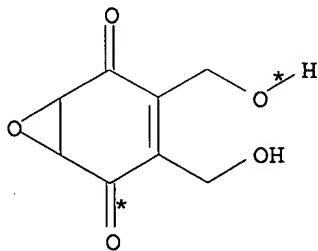
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

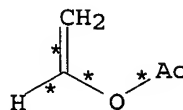
RX(117) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9)  
RX(117) 2 A + 2 B + 2 W + O ==> AJ



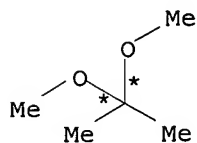
A



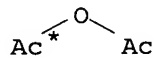
A



2 B



2 W

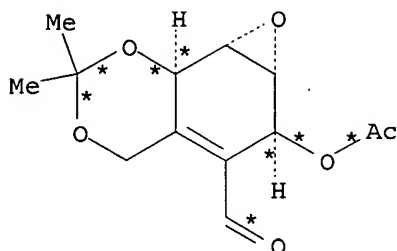


O

7  
STEPS  
→

Updated Search

10509228



AJ  
YIELD 87%

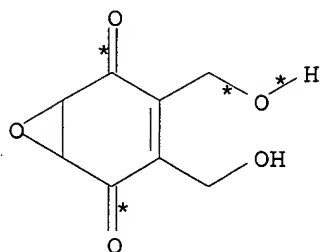
RX(1)	RCT A 556795-52-9, B 108-05-4 PRO C 676263-74-4 CAT 9001-62-1 Lipase SOL 1634-04-4 t-BuOMe CON 6 hours, 0 deg C NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
RX(3)	RCT C 676263-74-4 RGT M 1191-15-7 AlH(Bu-i) <sub>2</sub> PRO L 676263-76-6 SOL 109-99-9 THF CON -78 deg C NTE stereoselective
RX(6)	RCT L 676263-76-6, W 77-76-9 RGT Y 24057-28-1 Pyridinium tosylate PRO X 701921-77-9 SOL 67-64-1 Me <sub>2</sub> CO CON room temperature
RX(7)	RCT X 701921-77-9 RGT AA 16940-66-2 NaBH <sub>4</sub> PRO Z 701921-89-3 CAT 7790-86-5 CeCl <sub>3</sub> SOL 67-56-1 MeOH CON 0 deg C NTE stereoselective
RX(21)	RCT Z 701921-89-3 RGT AO 584-08-7 K <sub>2</sub> CO <sub>3</sub> PRO BB 701921-78-0, AD 701921-79-1 SOL 67-56-1 MeOH CON 0 deg C NTE stereoselective
RX(8)	RCT AD 701921-79-1 RGT AF 7782-44-7 O <sub>2</sub> , AG 7758-89-6 CuCl, AH 2564-83-2 Me <sub>4</sub> -piperidoxyl PRO AE 701921-80-4 SOL 68-12-2 DMF
RX(9)	RCT AE 701921-80-4, O 108-24-7 RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP

Updated Search

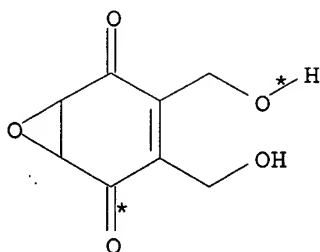
10509228

PRO AJ 701921-81-5  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

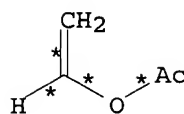
RX(118) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22)  
RX(118) 2 A + 2 B + 2 W + BC ==> BD



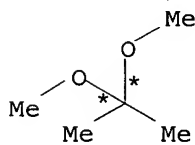
A



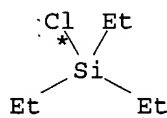
A



2 B

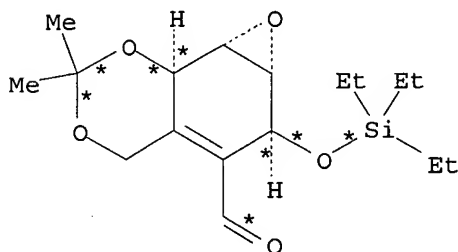


2 W



BC

7  
STEPS  
→



BD

YIELD 70%

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6

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SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

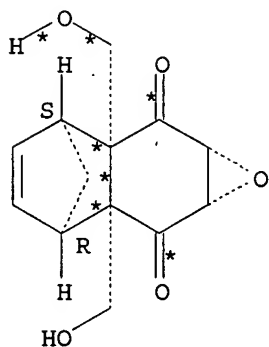
RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

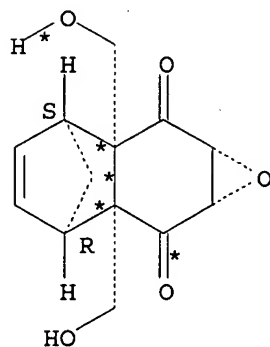
RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

RX(119) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
RX(9)

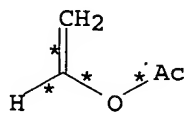
RX(119) 2 AX + 2 B + 2 W + O ==> AJ



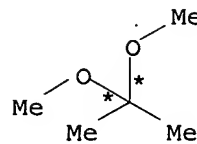
AX



AX



2 B



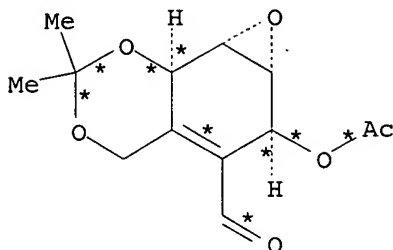
2 W

Updated Search



CC(=O)OCC(=O)C

8  
STEPS  
→



YIELD 87%

## Updated Search

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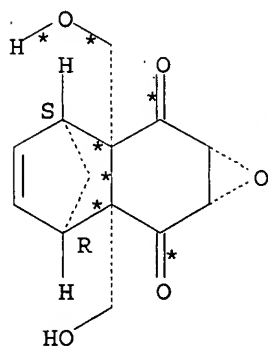
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

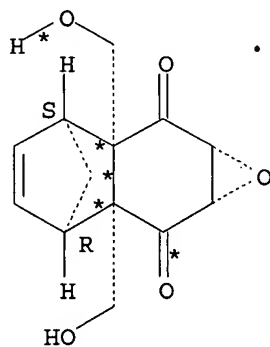
RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

RX(120) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
RX(22)

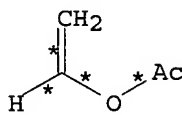
RX(120) 2 AX + 2 B + 2 W + BC ==> BD



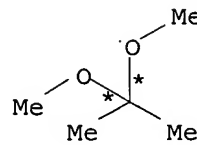
AX



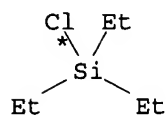
AX



2 B

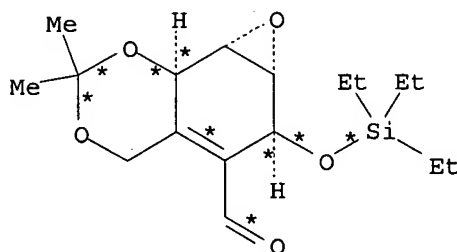


2 W



BC

8  
STEPS  
→



BD  
YIELD 70%

RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

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RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)2  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

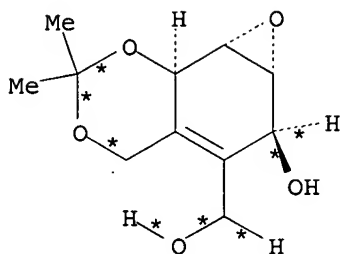
RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

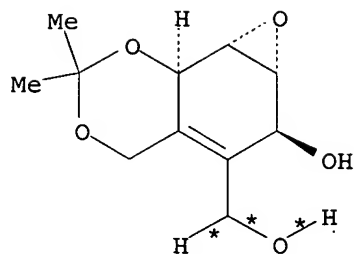
RX(155) OF 307 COMPOSED OF RX(8), RX(9), RX(10), RX(11), RX(13), RX(15), RX(17)  
RX(155) 2 AD + 2 O + 2 AK ==> T

Updated Search

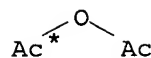
10509228



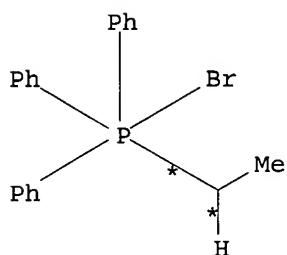
AD



AD

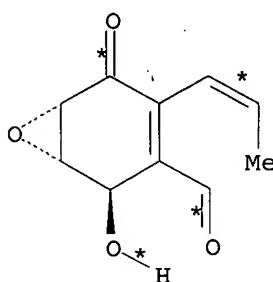


2 O



2 AK

7  
STEPS  
→



T

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K2CO3  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH2Cl2

Updated Search

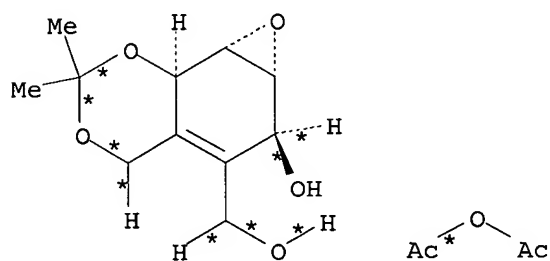
10509228

CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

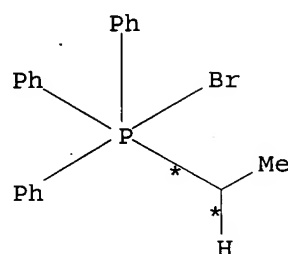
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(156) OF 307 COMPOSED OF RX(8), RX(9), RX(10), RX(11), RX(13), RX(12), RX(14)  
RX(156) AD + O + AK ==> AU



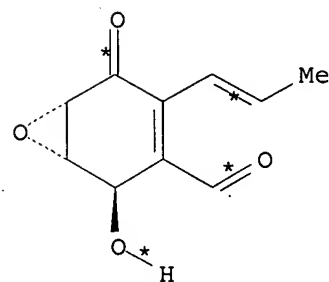
AD

O



AK

7  
STEPS  
→



AU

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5

Updated Search

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SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

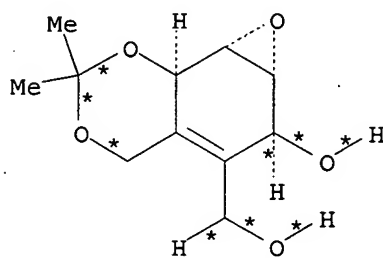
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

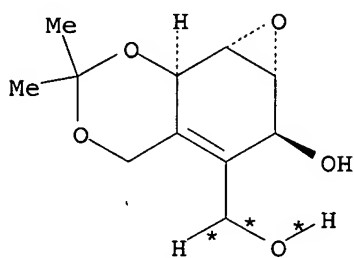
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(178) OF 307 COMPOSED OF RX(8), RX(22), RX(23), RX(24), RX(13), RX(15),  
RX(17)

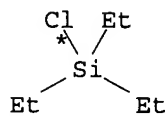
RX(178) 2 AD + BC + 2 AK ==> T



AD



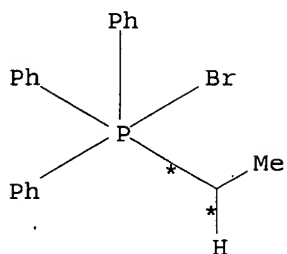
AD



BC

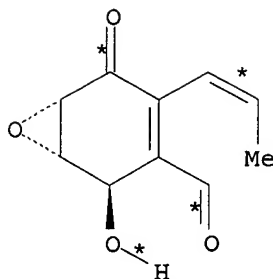
Updated Search

10509228



2 AK

7  
STEPS  
→



T

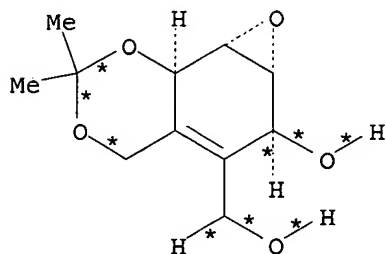
- RX(8): RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C
- RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective
- RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C
- RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield
- RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature
- RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

Updated Search

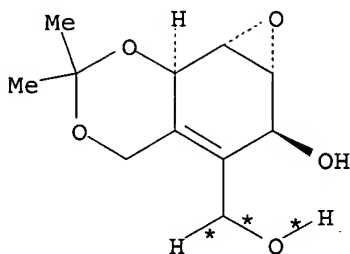
10509228

RX(179) OF 307 COMPOSED OF RX(8), RX(22), RX(23), RX(24), RX(13), RX(12),  
RX(14)

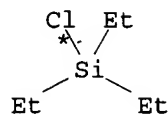
RX(179) 2 AD + BC + 2 AK ==> AU



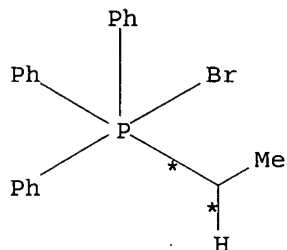
AD



AD

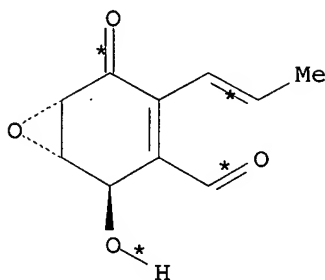


BC



2 AK

7  
STEPS  
→



AU

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF

Updated Search



10509228

CON 0 deg C

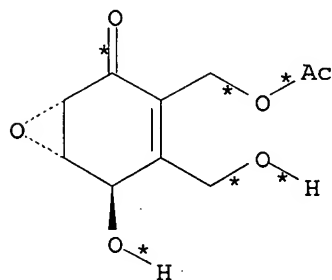
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

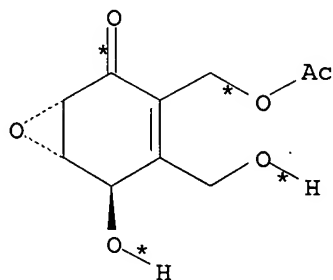
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(252) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9), RX(10), RX(11),  
RX(13), RX(15), RX(17)

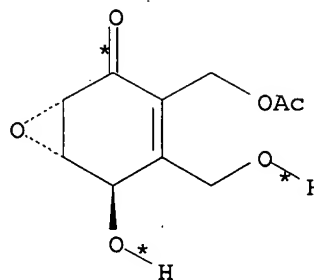
RX(252) 3 L + 3 W + 2 O + 2 AK ==> T



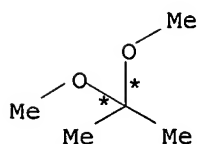
L



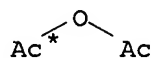
L



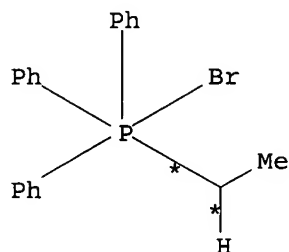
L



3 W



2 O

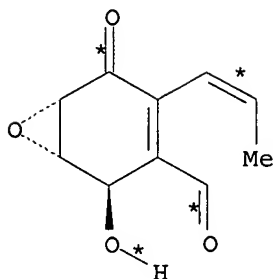


2 AK

10  
STEPS  
→

Updated Search

10509228



T

RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me <sub>2</sub> CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH <sub>4</sub>
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl <sub>3</sub>
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(21)	RCT	Z 701921-89-3
	RGT	AO 584-08-7 K <sub>2</sub> CO <sub>3</sub>
	PRO	BB 701921-78-0, AD 701921-79-1
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(8)	RCT	AD 701921-79-1
	RGT	AF 7782-44-7 O <sub>2</sub> , AG 7758-89-6 CuCl, AH 2564-83-2
		Me <sub>4</sub> -piperidoxyl
	PRO	AE 701921-80-4
	SOL	68-12-2 DMF
RX(9)	RCT	AE 701921-80-4, O 108-24-7
	RGT	Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
	PRO	AJ 701921-81-5
	SOL	75-09-2 CH <sub>2</sub> Cl <sub>2</sub>
	CON	0 deg C
RX(10)	RCT	AJ 701921-81-5, AK 154489-89-1
	RGT	AM 109-72-8 BuLi
	PRO	AL 701921-82-6
	SOL	109-99-9 THF
	CON	0 deg C
	NTE	stereoselective
RX(11)	RCT	AL 701921-82-6
	RGT	AO 584-08-7 K <sub>2</sub> CO <sub>3</sub>
	PRO	AN 701921-92-8
	SOL	67-56-1 MeOH

Updated Search

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CON 0 deg C

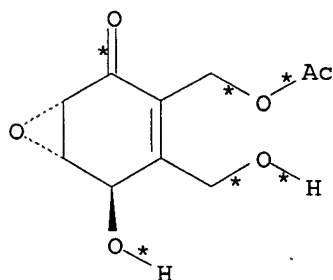
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

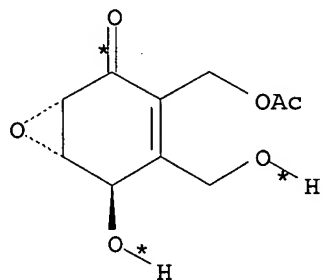
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(253) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9), RX(10), RX(11),  
RX(13), RX(12), RX(14)

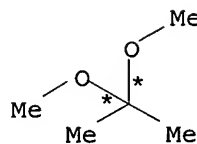
RX(253) 2 L + 2 W + O + AK ==> AU



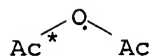
L



L



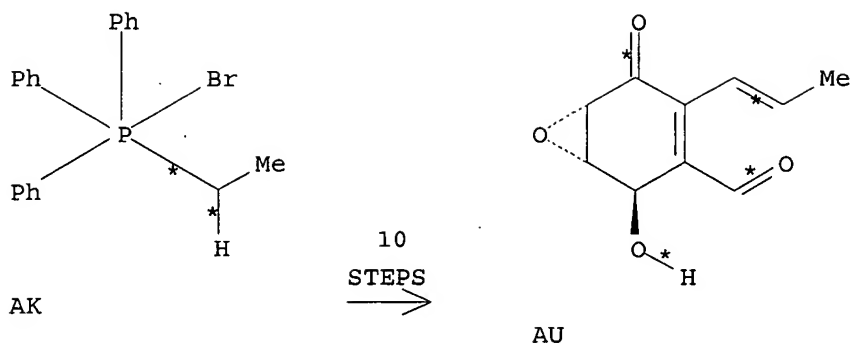
2 W



O

Updated Search

10509228



RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH

Updated Search

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CON 0 deg C

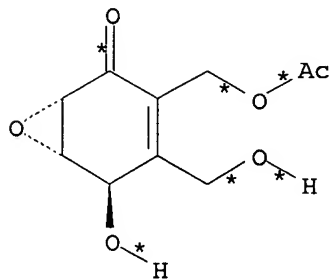
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

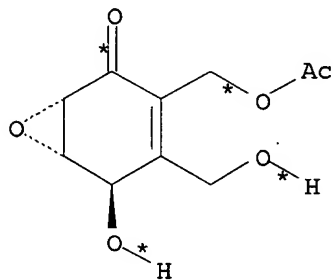
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(254) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22), RX(23), RX(24),  
RX(13), RX(15), RX(17)

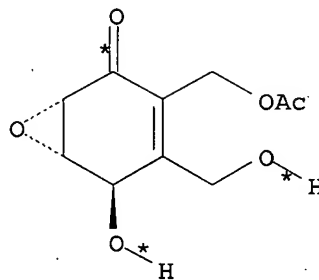
RX(254) 3 L + 3 W + 2 BC + 2 AK ==> T



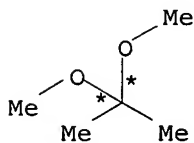
L



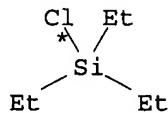
L



L



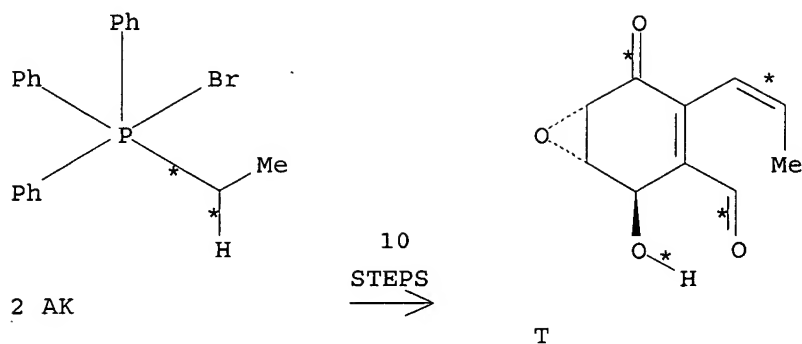
3 W



2 BC

Updated Search

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- RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature
- RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C
- RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective
- RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF

Updated Search

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CON 0 deg C

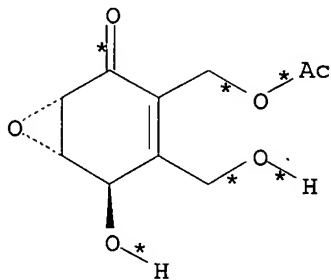
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

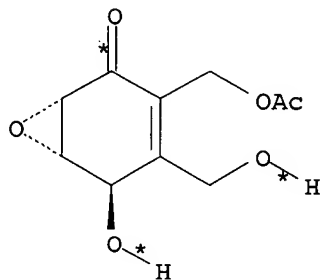
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(255) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22), RX(23), RX(24),  
RX(13), RX(12), RX(14)

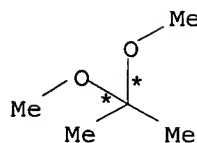
RX(255) 2 L + 2 W + BC + AK ==> AU



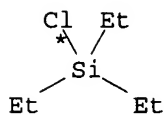
L



L



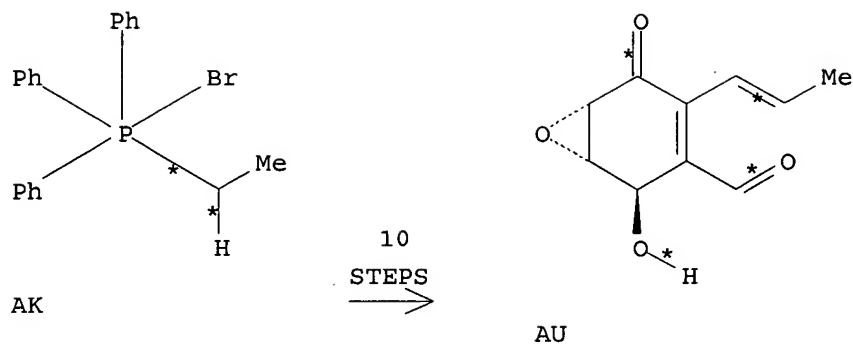
2 W



BC

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- RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature
- RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C
- RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective
- RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF

Updated Search



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CON 0 deg C

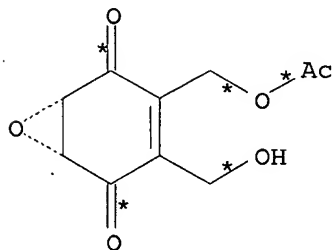
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

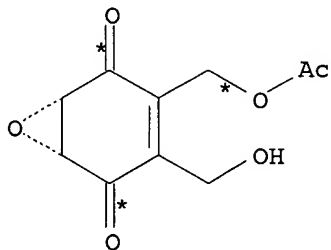
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(256) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9), RX(10),  
RX(11), RX(13), RX(15), RX(17)

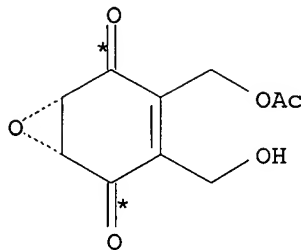
RX(256) 3 C + 3 W + 2 O + 2 AK ==> T



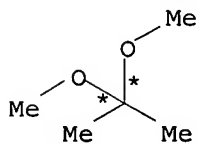
C



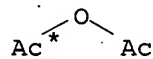
C



C



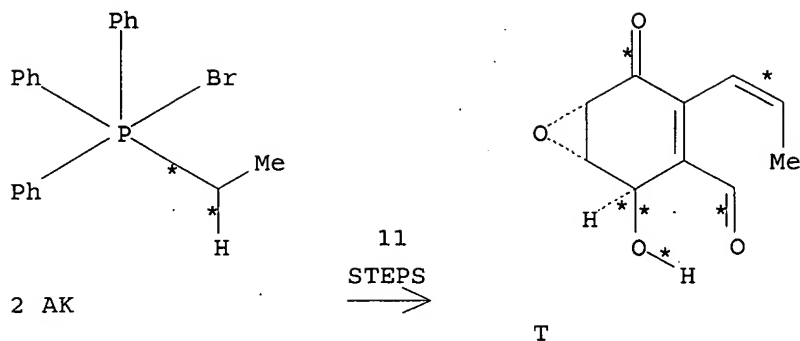
3 W



2 O

Updated Search

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- RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective
- RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature
- RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C
- RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF

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CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

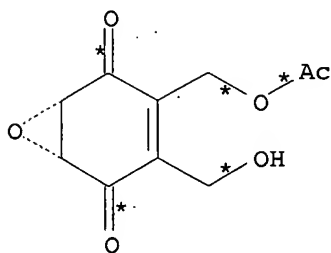
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

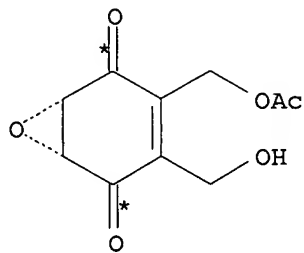
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(257) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9), RX(10),  
RX(11), RX(13), RX(12), RX(14)

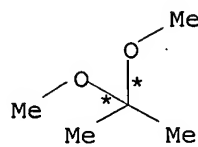
RX(257) 2 C + 2 W + O + AK ==> AU



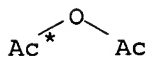
C



C



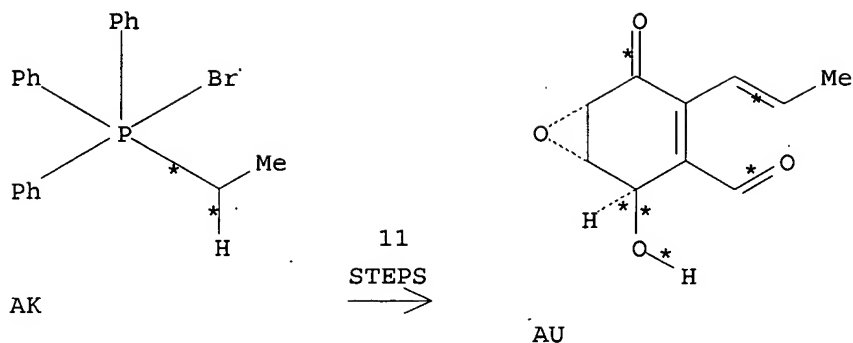
2 W



O

Updated Search

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- RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective
- RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature
- RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C
- RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF

Updated Search

10509228

CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

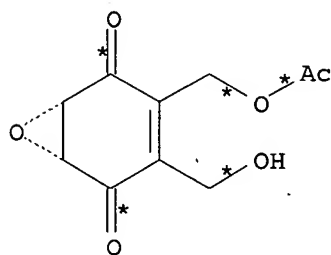
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

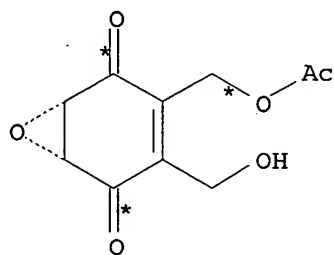
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(258) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22), RX(23),  
RX(24), RX(13), RX(15), RX(17)

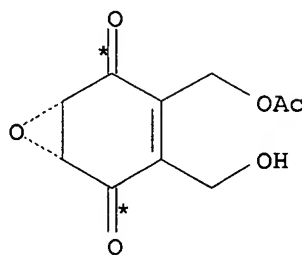
RX(258) 3 C + 3 W + 2 BC + 2 AK ==> T



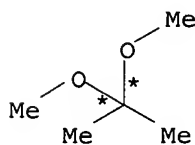
C



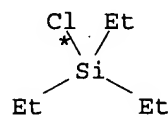
C



C



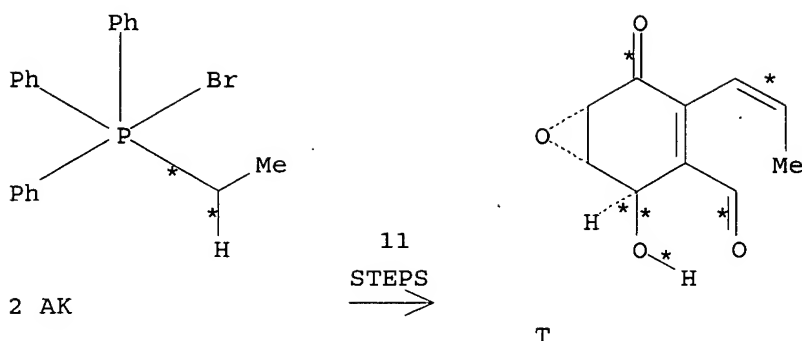
3 W



2 BC

Updated Search

10509228



RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF

Updated Search

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CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

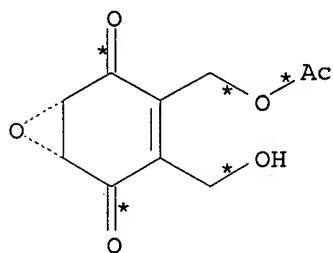
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

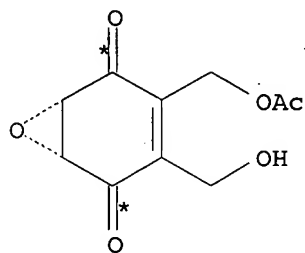
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(259) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22), RX(23),  
RX(24), RX(13), RX(12), RX(14)

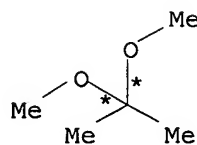
RX(259) 2 C + 2 W + BC + AK ==> AU



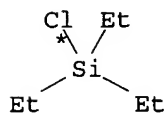
C



C



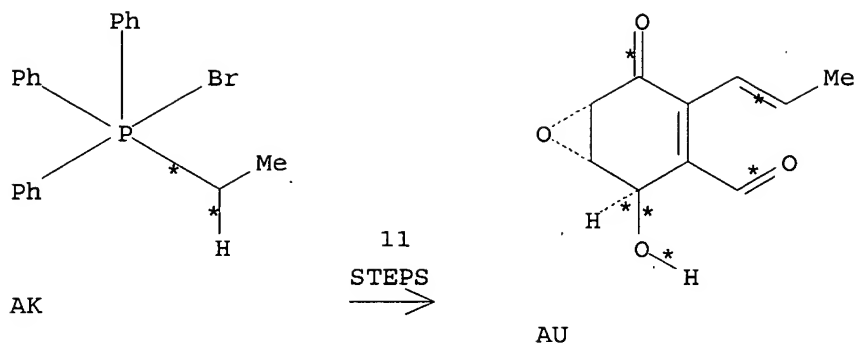
2 W



BC

Updated Search

10509228



RX (3)	RCT C 676263-74-4
	RGT M 1191-15-7 AlH(Bu-i) <sub>2</sub>
	PRO L 676263-76-6
	SOL 109-99-9 THF
	CON -78 deg C
	NTE stereoselective
RX (6)	RCT L 676263-76-6, W 77-76-9
	RGT Y 24057-28-1 Pyridinium tosylate
	PRO X 701921-77-9
	SOL 67-64-1 Me <sub>2</sub> CO
	CON room temperature
RX (7)	RCT X 701921-77-9
	RGT AA 16940-66-2 NaBH <sub>4</sub>
	PRO Z 701921-89-3
	CAT 7790-86-5 CeCl <sub>3</sub>
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX (21)	RCT Z 701921-89-3
	RGT AO 584-08-7 K <sub>2</sub> CO <sub>3</sub>
	PRO BB 701921-78-0, AD 701921-79-1
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX (8)	RCT AD 701921-79-1
	RGT AF 7782-44-7 O <sub>2</sub> , AG 7758-89-6 CuCl, AH 2564-83-2 Me <sub>4</sub> -piperidoxyl
	PRO AE 701921-80-4
	SOL 68-12-2 DMF
RX (22)	RCT AE 701921-80-4, BC 994-30-9
	RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
	PRO BD 701921-90-6
	SOL 75-09-2 CH <sub>2</sub> Cl <sub>2</sub>
	CON 0 deg C
RX (23)	RCT BD 701921-90-6, AK 154489-89-1
	RGT AM 109-72-8 BuLi
	PRO BF 701921-91-7
	SOL 109-99-9 THF

Updated Search



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CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

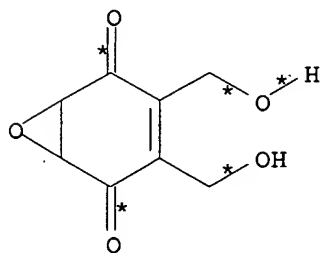
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

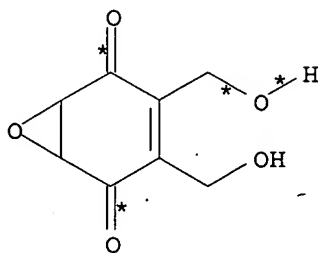
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(260) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9),  
RX(10), RX(11), RX(13), RX(15), RX(17)

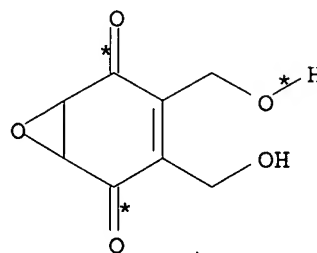
RX(260) 3 A + 3 B + 3 W + 2 O + 2 AK ==> T



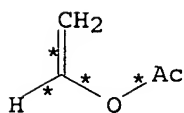
A



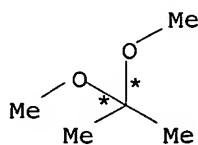
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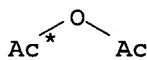
A



3 B



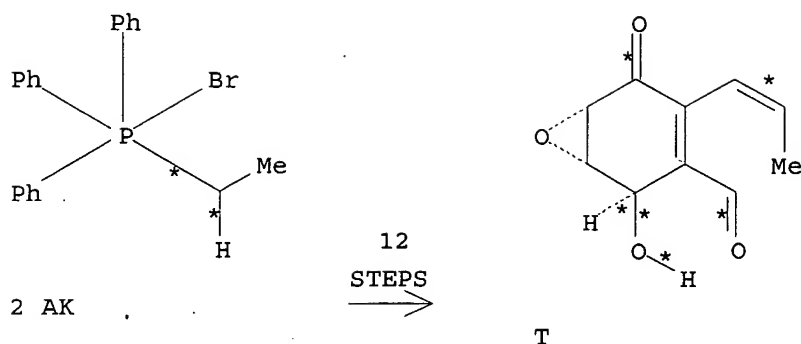
3 W



2 O

Updated Search

10509228



- RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
- RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective
- RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature
- RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective
- RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF
- RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP

Updated Search

10509228

PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

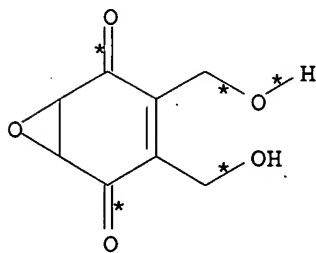
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

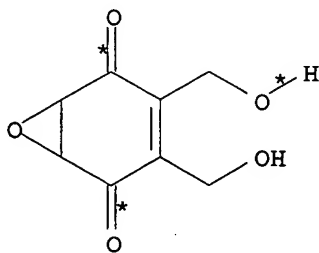
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(261) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9),  
RX(10), RX(11), RX(13), RX(12), RX(14)

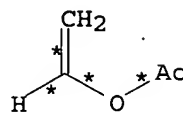
RX(261) 2 A + 2 B + 2 W + O + AK ==> AU



A



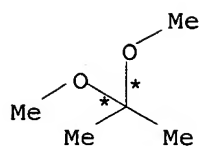
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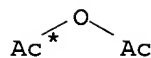
2 B

Updated Search

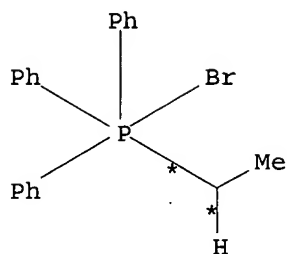
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2 W

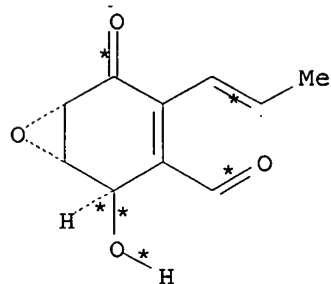


O



AK

12  
STEPS  
→



AU

- RX(1) RCT A 556795-52-9, B 108-05-4  
 PRO C 676263-74-4  
 CAT 9001-62-1 Lipase  
 SOL 1634-04-4 t-BuOMe  
 CON 6 hours, 0 deg C  
 NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
- RX(3) RCT C 676263-74-4  
 RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
 PRO L 676263-76-6  
 SOL 109-99-9 THF  
 CON -78 deg C  
 NTE stereoselective
- RX(6) RCT L 676263-76-6, W 77-76-9  
 RGT Y 24057-28-1 Pyridinium tosylate  
 PRO X 701921-77-9  
 SOL 67-64-1 Me<sub>2</sub>CO  
 CON room temperature
- RX(7) RCT X 701921-77-9  
 RGT AA 16940-66-2 NaBH<sub>4</sub>  
 PRO Z 701921-89-3  
 CAT 7790-86-5 CeCl<sub>3</sub>  
 SOL 67-56-1 MeOH  
 CON 0 deg C  
 NTE stereoselective

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RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

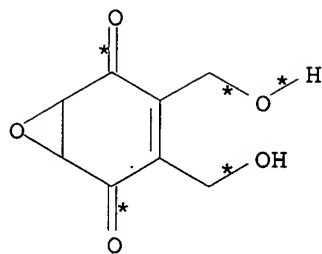
RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

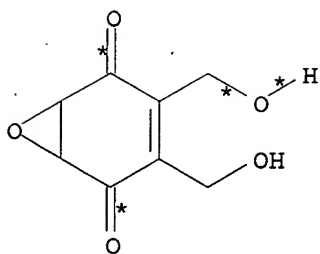
RX(262) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22),  
RX(23), RX(24), RX(13), RX(15), RX(17)  
RX(262) 3 A + 3 B + 3 W + 2 BC + 2 AK ==> T

Updated Search

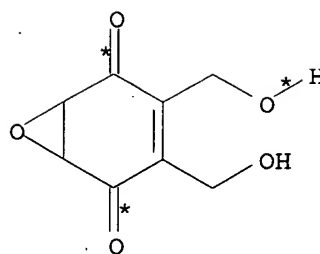
10509228



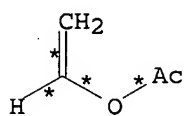
A



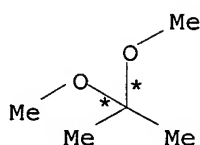
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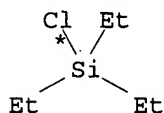
A



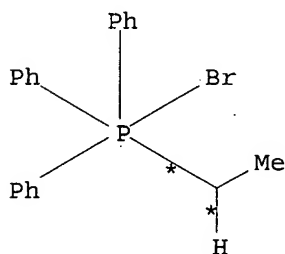
3 B



3 W

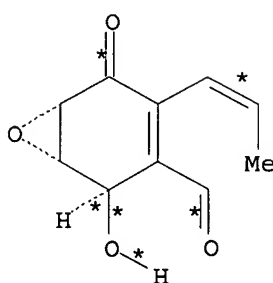


2 BC



2 AK

12  
STEPS  
→



T

RX(1) RCT A 556795-52-9, B 108-05-4  
 PRO C 676263-74-4  
 CAT 9001-62-1 Lipase  
 SOL 1634-04-4 t-BuOMe  
 CON 6 hours, 0 deg C  
 NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective

RX(3) RCT C 676263-74-4  
 RGT M 1191-15-7 AlH(Bu-i)2  
 PRO L 676263-76-6  
 SOL 109-99-9 THF  
 CON -78 deg C  
 NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
 RGT Y 24057-28-1 Pyridinium tosylate  
 PRO X 701921-77-9  
 SOL 67-64-1 Me2CO  
 CON room temperature

Updated Search

10509228

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

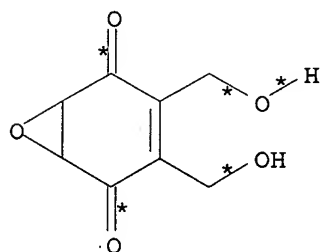
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF

Updated Search

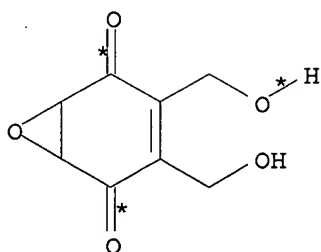
10509228

CON room temperature

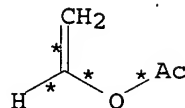
RX(263) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22),  
RX(23), RX(24), RX(13), RX(12), RX(14)  
RX(263) 2 A + 2 B + 2 W + BC + AK ==> AU



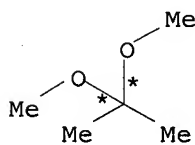
A



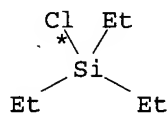
A



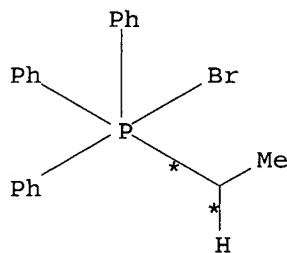
2 B



2 W

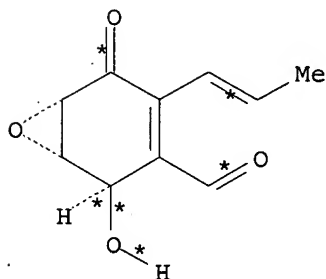


BC



AK

12  
STEPS  
→



AU

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

Updated Search



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RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

Updated Search

10509228

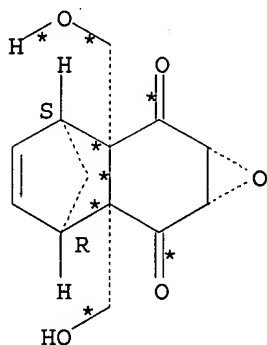
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

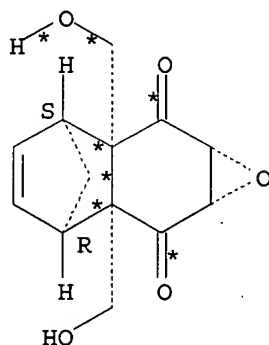
RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

RX(264) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
RX(9), RX(10), RX(11), RX(13), RX(15), RX(17)

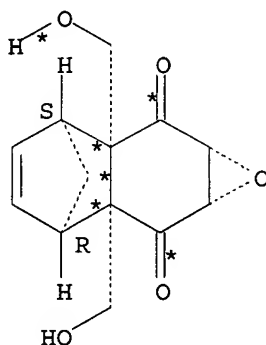
RX(264) 3 AX + 3 B + 3 W + 2 O + 2 AK ==> T



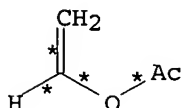
AX



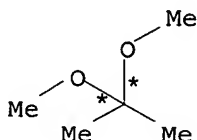
AX



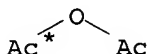
AX



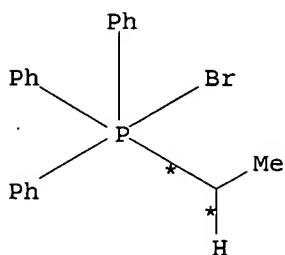
3 B



3 W

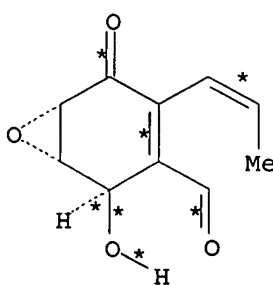


2 O



2 AK

13  
STEPS  
→



T

Updated Search

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RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C

Updated Search

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NTE stereoselective

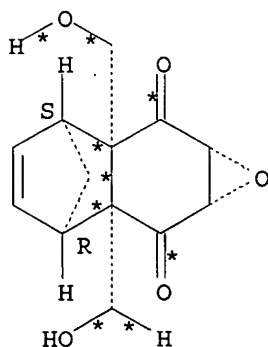
RX(11) RCT AL 701921-82-6  
 RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO AN 701921-92-8  
 SOL 67-56-1 MeOH  
 CON 0 deg C

RX(13) RCT AN 701921-92-8  
 RGT AT 20039-37-6 PDC  
 PRO AS 701921-84-8, AP 701921-83-7  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 0 deg C  
 NTE stereoselective, 81% overall yield

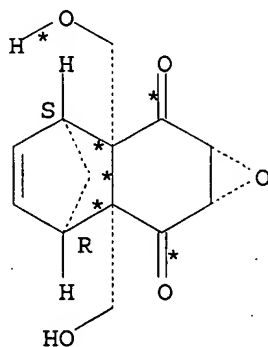
RX(15) RCT AS 701921-84-8  
 RGT AR 9037-24-5 Amberlyst 15  
 PRO AV 701921-85-9  
 SOL 67-56-1 MeOH  
 CON room temperature

RX(17) RCT AV 701921-85-9  
 RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
 Me<sub>4</sub>-piperidoxyl  
 PRO T 701921-87-1  
 SOL 68-12-2 DMF  
 CON room temperature

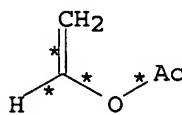
RX(265) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
 RX(9), RX(10), RX(11), RX(13), RX(12), RX(14)  
 RX(265) 2 AX + 2 B + 2 W + O + AK ==> AU



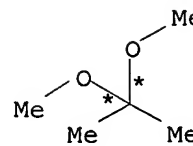
AX



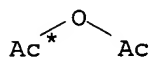
AX



2 B



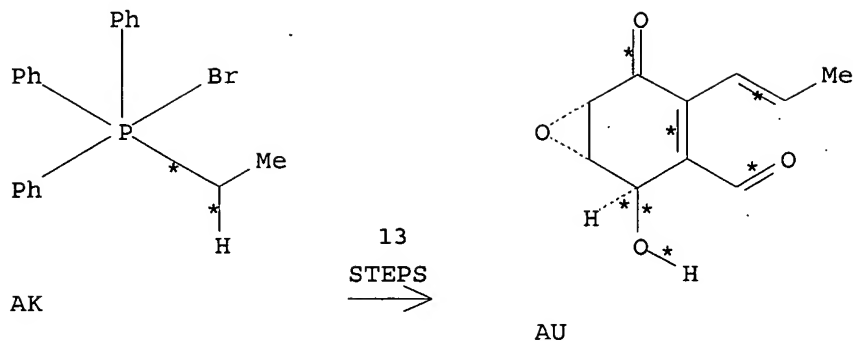
2 W



O

Updated Search

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RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2 Me<sub>4</sub>-piperidoxyl

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PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7  
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP  
PRO AJ 701921-81-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO AL 701921-82-6  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(11) RCT AL 701921-82-6  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AN 701921-92-8  
SOL 67-56-1 MeOH  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

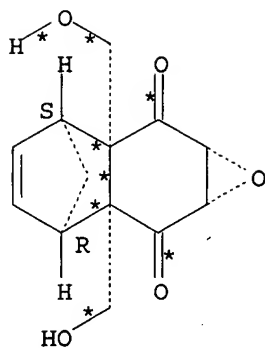
RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

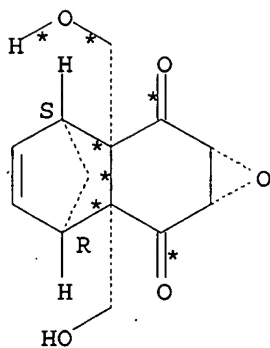
RX(266) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
RX(22), RX(23), RX(24), RX(13), RX(15), RX(17)

RX(266) 3 AX + 3 B + 3 W + 2 BC + 2 AK ==> T

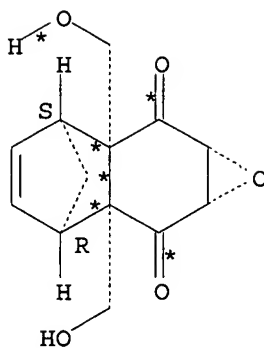
10509228



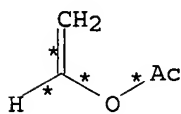
AX



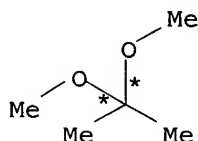
AX



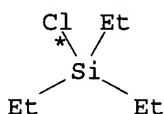
AX



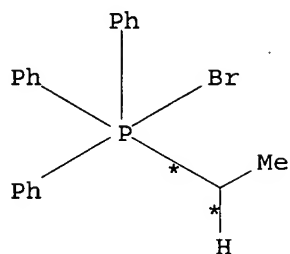
3 B



3 W

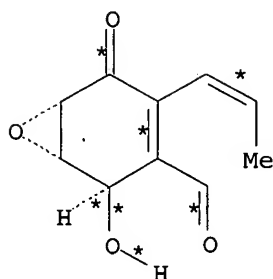


2 BC



2 AK

13  
STEPS  
→



T

RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4

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PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me<sub>2</sub>CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH<sub>4</sub>  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl<sub>3</sub>  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

Updated Search



10509228

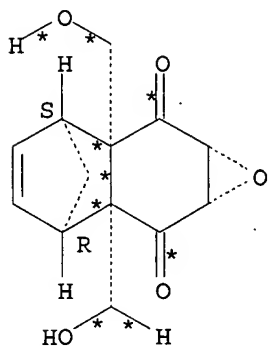
RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8  
RGT AR 9037-24-5 Amberlyst 15  
PRO AV 701921-85-9  
SOL 67-56-1 MeOH  
CON room temperature

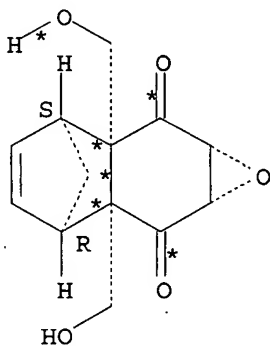
RX(17) RCT AV 701921-85-9  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO T 701921-87-1  
SOL 68-12-2 DMF  
CON room temperature

RX(267) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),  
RX(22), RX(23), RX(24), RX(13), RX(12), RX(14)

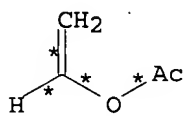
RX(267) 2 AX + 2 B + 2 W + BC + AK ==> AU



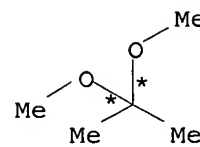
AX



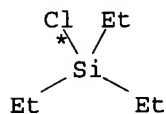
AX



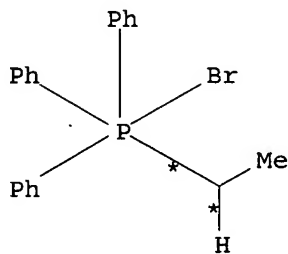
2 B



2 W

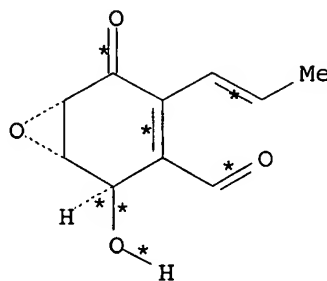


BC



AK

13  
STEPS  
→



AU

Updated Search

10509228

RX(19) RCT AX 556795-51-8  
PRO A 556795-52-9  
SOL 101-84-8 PhOPh  
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4  
PRO C 676263-74-4  
CAT 9001-62-1 Lipase  
SOL 1634-04-4 t-BuOMe  
CON 6 hours, 0 deg C  
NTE biotransformation, enzymic, lipase PS 30(amino) used,  
stereoselective

RX(3) RCT C 676263-74-4  
RGT M 1191-15-7 AlH(Bu-i)2  
PRO L 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
PRO X 701921-77-9  
SOL 67-64-1 Me2CO  
CON room temperature

RX(7) RCT X 701921-77-9  
RGT AA 16940-66-2 NaBH4  
PRO Z 701921-89-3  
CAT 7790-86-5 CeCl3  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(21) RCT Z 701921-89-3  
RGT AO 584-08-7 K2CO3  
PRO BB 701921-78-0, AD 701921-79-1  
SOL 67-56-1 MeOH  
CON 0 deg C  
NTE stereoselective

RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2  
Me4-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9  
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP  
PRO BD 701921-90-6  
SOL 75-09-2 CH2Cl2  
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1  
RGT AM 109-72-8 BuLi  
PRO BF 701921-91-7  
SOL 109-99-9 THF  
CON 0 deg C  
NTE stereoselective

Updated Search

10509228

RX(24) RCT BF 701921-91-7  
RGT BG 62778-11-4 Olah's reagent  
PRO AN 701921-92-8  
SOL 109-99-9 THF  
CON 0 deg C

RX(13) RCT AN 701921-92-8  
RGT AT 20039-37-6 PDC  
PRO AS 701921-84-8, AP 701921-83-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7  
RGT AR 9037-24-5 Amberlyst 15  
PRO AQ 494196-00-8  
SOL 67-56-1 MeOH  
CON room temperature

RX(14) RCT AQ 494196-00-8  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AU 701921-86-0  
SOL 68-12-2 DMF  
CON room temperature

L3 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:339244 CASREACT  
TITLE: Benzimidazolone p38 inhibitors  
AUTHOR(S): Dombroski, Mark A.; Letavic, Michael A.; McClure, Kim  
F.; Barberia, John T.; Carty, Thomas J.; Cortina,  
Santo R.; Csiki, Csilla; Dipesa, Alan J.; Elliott,  
Nancy C.; Gabel, Christopher A.; Jordan, Crystal K.;  
Labasi, Jeff M.; Martin, William H.; Peese, Kevin M.;  
Stock, Ingrid A.; Svensson, Linne; Sweeney, Francis  
J.; Yu, Chul H.  
CORPORATE SOURCE: Pfizer Global Research and Development, Groton  
Laboratories, Groton, CT, 06340, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),  
14(4), 919-923  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

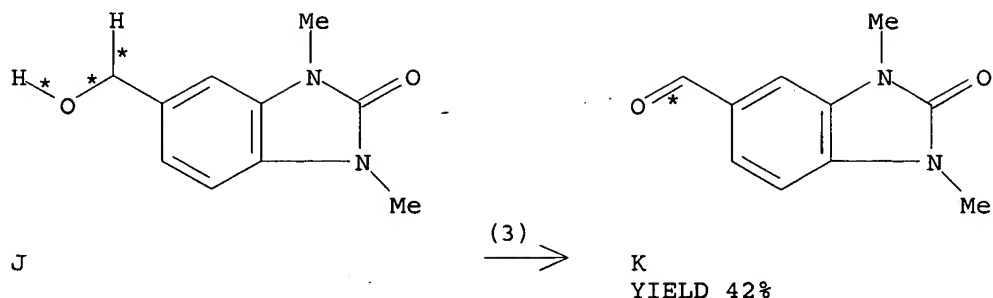
AB The synthesis and in vitro p38 $\alpha$  activity of a novel series of  
benzimidazolone inhibitors is described. The p38 $\alpha$  SAR is consistent  
with a mode of binding wherein the benzimidazolone carbonyl serves as the  
H-bond acceptor to Met109 of p38 $\alpha$  in a manner analogous to the  
pyridine nitrogen of prototypical pyridylimidazole p38 inhibitors. Potent  
p38 $\alpha$  activity comparable to that of several previously reported p38  
inhibitors is observed for this novel chemotype.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 443 ...J ==> K...

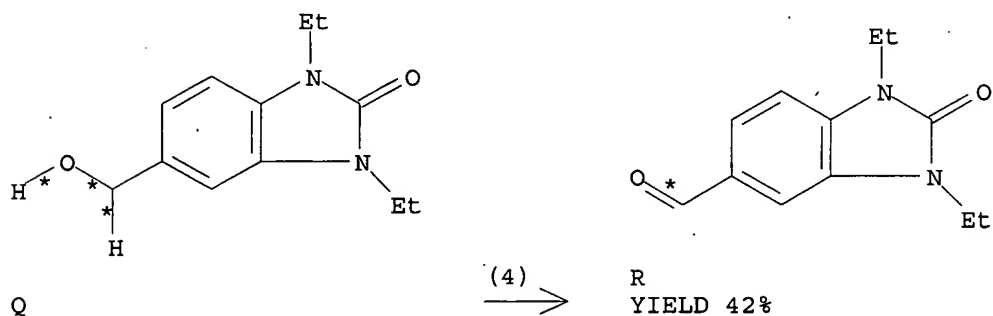
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RX(3) RCT J 345657-96-7  
RGT L 2564-83-2 Me4-piperidoxyl, M 128-09-6  
Chlorosuccinimide  
PRO K 55241-49-1  
CAT 1112-67-0 Bu4NCl  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 5.5 hours, room temperature, pH 8.6  
NTE buffered soln.

RX(4) OF 443 ...Q ==> R...



RX(4) RCT Q 864512-93-6  
RGT L 2564-83-2 Me4-piperidoxyl, M 128-09-6  
Chlorosuccinimide  
PRO R 14624-85-2  
CAT 1112-67-0 Bu4NCl  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 5.5 hours, room temperature, pH 8.6  
NTE buffered soln.

L3 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 140:321153 CASREACT  
TITLE: Enantioselective total synthesis of  
(+)-panepophenanthrin, a novel inhibitor of the  
ubiquitin-activating enzyme  
AUTHOR(S): Mehta, Goverdhan; Ramesh, Senaiar S.  
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of  
Science, Bangalore, 560 012, India  
SOURCE: Tetrahedron Letters (2004), 45(9), 1985-1987

Updated Search

10509228

PUBLISHER:  
DOCUMENT TYPE:  
LANGUAGE:  
GI

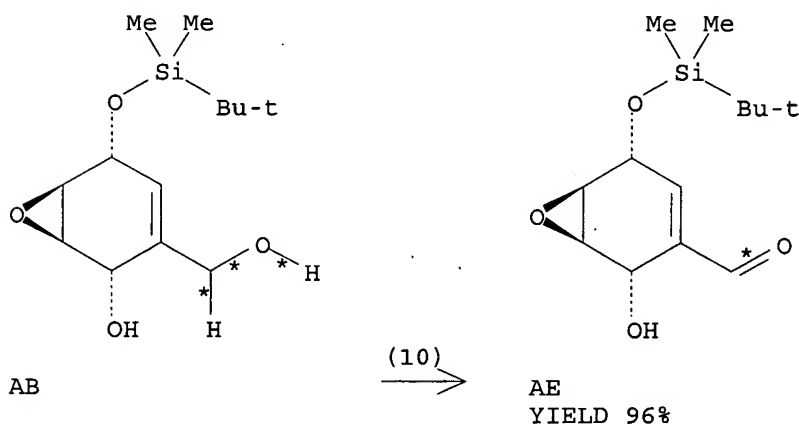
CODEN: TELEAY; ISSN: 0040-4039  
Elsevier Science B.V.  
Journal  
English

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB An enantioselective total synthesis of the novel natural product (+)-panepophenanthrin (I) has been accomplished in which a biomimetic Diels-Alder dimerization is a key step. The monomeric precursor II was assembled from the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone through a short, simple sequence employing chemo- and stereoselective operations.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(10) OF 115 ...AB ==> AE...

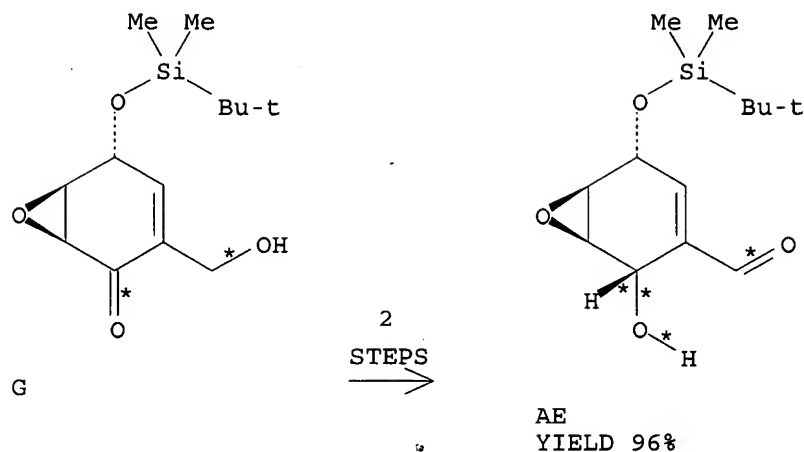


RX(10) RCT AB 678197-28-9  
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH  
7758-89-6 CuCl  
PRO AE 678197-29-0  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(23) OF 115 COMPOSED OF RX(9), RX(10)  
RX(23) G ==> AE

Updated Search

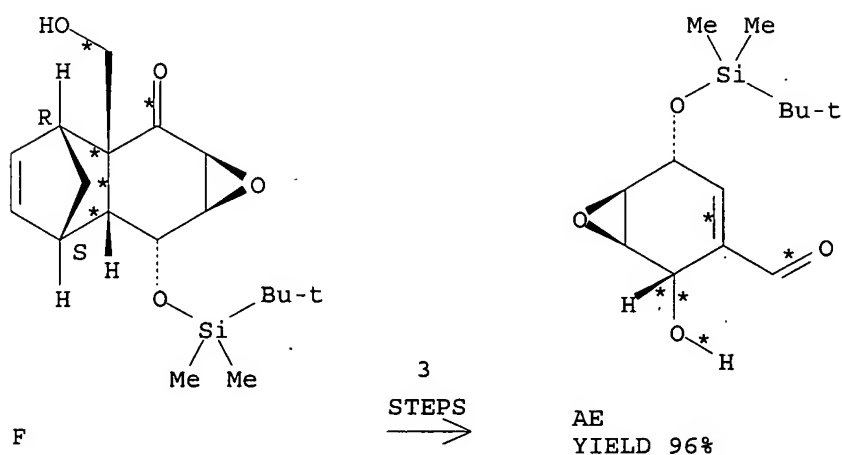
10509228



RX(9) RCT G 678197-25-6  
RGT AC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO AB 678197-28-9  
SOL 109-99-9 THF, 110-54-3 Hexane  
CON 10 minutes, -78 deg C  
NTE stereoselective

RX(10) RCT AB 678197-28-9  
RGT AF 2564-83-2 Me<sub>4</sub>-piperidoxyl, AG 7782-44-7 O<sub>2</sub>, AH  
7758-89-6 CuCl  
PRO AE 678197-29-0  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(30) OF 115 COMPOSED OF RX(3), RX(9), RX(10)  
RX(30) F ==> AE



RX(3) RCT F 678197-27-8  
PRO G 678197-25-6

Updated Search

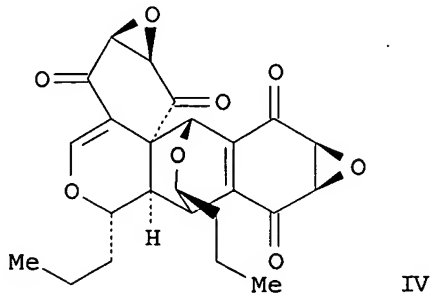
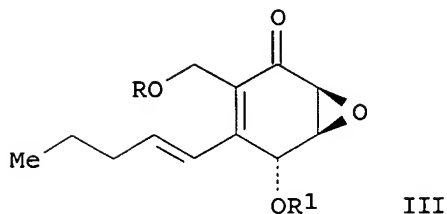
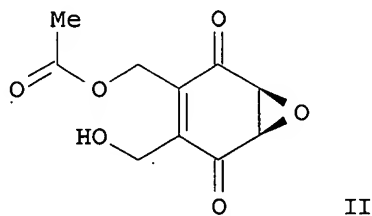
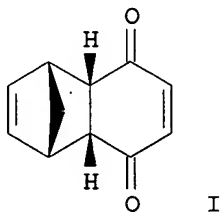
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SOL 101-84-8 PhOPh  
CON 240 deg C

RX(9) RCT G 678197-25-6  
RGT AC 1191-15-7 AlH(Bu-i)2  
PRO AB 678197-28-9  
SOL 109-99-9 THF, 110-54-3 Hexane  
CON 10 minutes, -78 deg C  
NTE stereoselective

RX(10) RCT AB 678197-28-9  
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH  
7758-89-6 CuCl  
PRO AE 678197-29-0  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

L3 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 140:287206 CASREACT  
TITLE: Total Synthesis of the Novel NF- $\kappa$ B Inhibitor  
(-)-Cycloepoxydon  
AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul  
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of  
Science, Bangalore, 560 012, India  
SOURCE: Organic Letters (2004), 6(5), 807-810  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB An enantioselective total synthesis of the novel, biol. active epoxyquinone natural product (-)-cycloepoxydon has been accomplished from

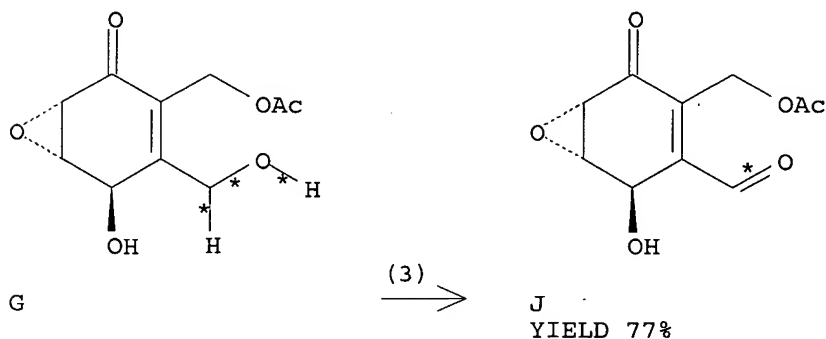
Updated Search

10509228

the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone I. Epoxyquinone II, derived from I, was transformed into pentenyl epoxy acetate III (R = R1 = COMe), which was hydrolyzed and protected to give III (R = SiMe2CMe3, R1 = H). The latter compound underwent epoxidn. of the linear chain alkene and deprotection to give the title compound. A new cycloepoxydon related heptacyclic dimer IV has also been prepared from III (R = SiMe2CMe3, R1 = H) and characterized.

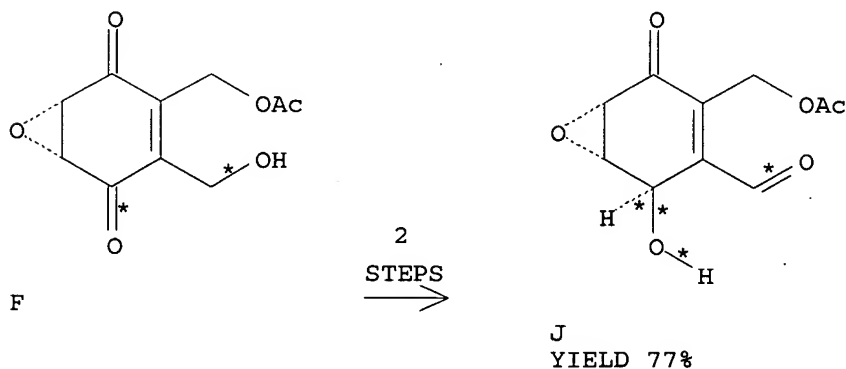
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 100 ...G ==> J...



RX(3) RCT G 676263-76-6  
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2  
PRO J 676263-78-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(13) OF 100 COMPOSED OF RX(2), RX(3)  
RX(13) F ==> J



RX(2) RCT F 676263-74-4  
RGT H 1191-15-7 AlH(Bu-i)2  
PRO G 676263-76-6

Updated Search

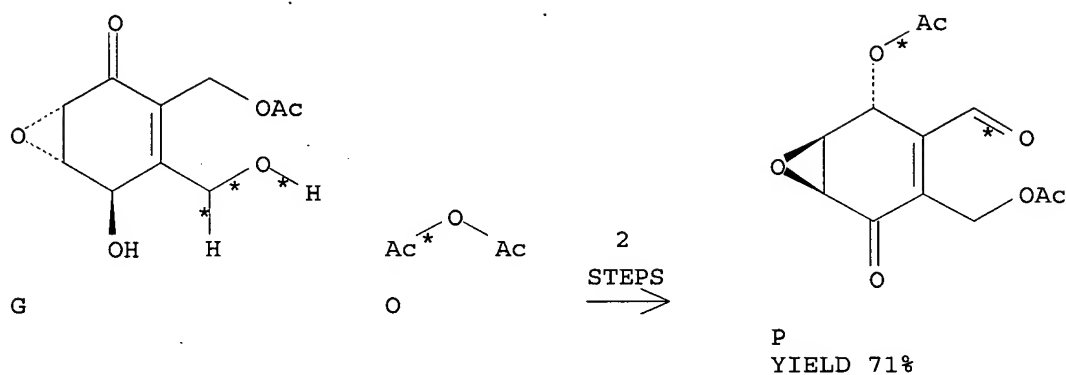


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SOL 109-99-9 THF  
CON -78 deg C  
NTE regioselective, stereoselective

RX(3) RCT G 676263-76-6  
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2  
PRO J 676263-78-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(14) OF 100 COMPOSED OF RX(3), RX(4)  
RX(14) G + O ==> P



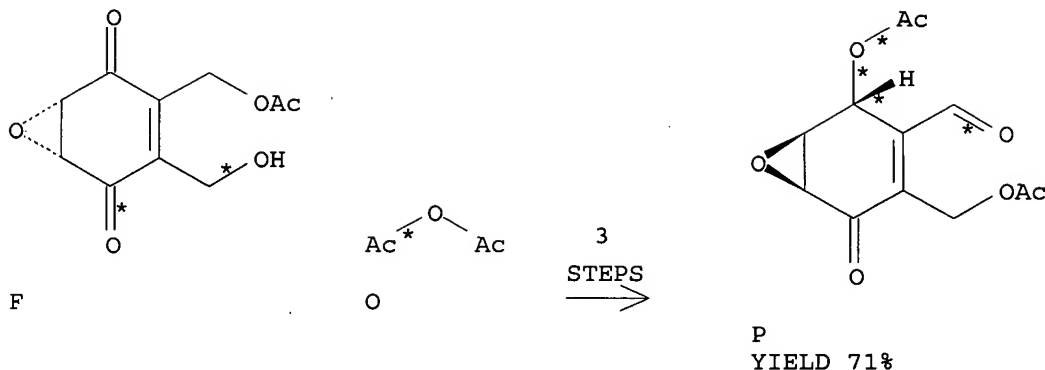
RX(3) RCT G 676263-76-6  
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2  
PRO J 676263-78-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(4) RCT J 676263-78-8, O 108-24-7  
RGT Q 110-86-1 Pyridine  
PRO P 676263-80-2  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON 0 deg C  
NTE stereoselective

RX(25) OF 100 COMPOSED OF RX(2), RX(3), RX(4)  
RX(25) F + O ==> P

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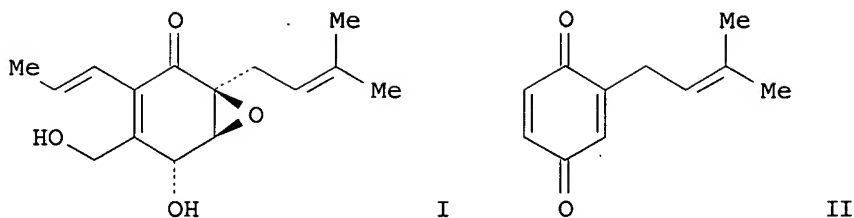
RX(2) RCT F 676263-74-4  
RGT H 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO G 676263-76-6  
SOL 109-99-9 THF  
CON -78 deg C  
NTE regioselective, stereoselective

RX(3) RCT G 676263-76-6  
RGT K 2564-83-2 Me<sub>4</sub>-piperidoxyl, L 7782-44-7 O<sub>2</sub>  
PRO J 676263-78-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

RX(4) RCT J 676263-78-8, O 108-24-7  
RGT Q 110-86-1 Pyridine  
PRO P 676263-80-2  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C  
NTE stereoselective

L3 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 140:270655 CASREACT  
TITLE: Total Synthesis of the Novel Antifungal Agent  
(±)-Jesterone  
AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra  
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of  
Science, Bangalore, 560 012, India  
SOURCE: Organic Letters (2004), 6(5), 811-813  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

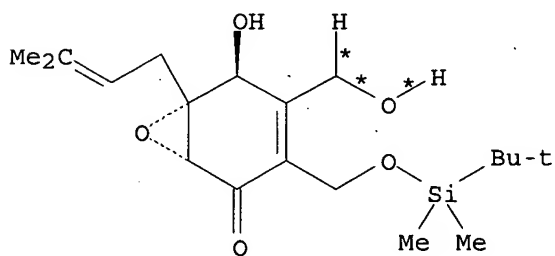
10509228



AB A total synthesis of the novel, biol. active epoxyquinone natural product (+)-jesterone (I) was accomplished via the formation of the Diels-Alder adduct of cyclopentadiene and prenylated 1,4-benzoquinone II. This approach is notable for its conceptual simplicity and efficient orchestration of a series of chemo-, regio-, and stereoselective operations.

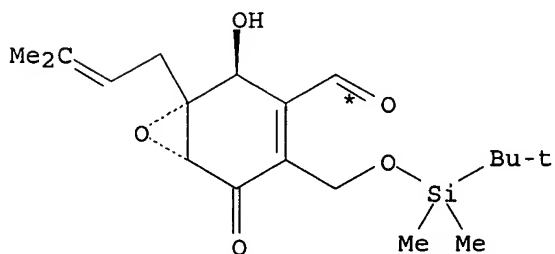
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 201 ...AF ==> AH...



AF

(11) →



AH  
YIELD 90%

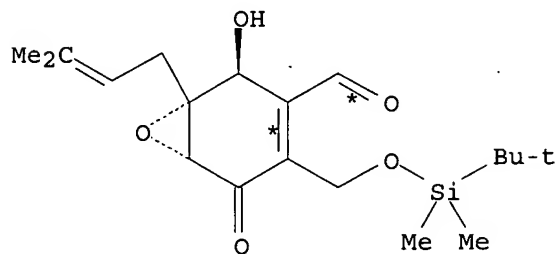
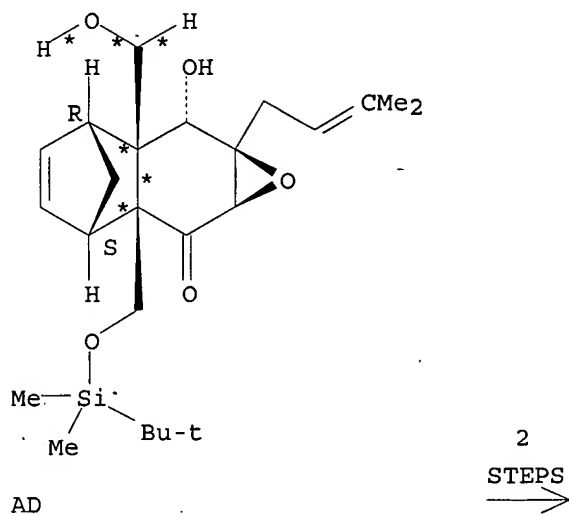
RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF

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10509228

CON 3 hours, room temperature  
NTE chemoselective

RX(26) OF 201 COMPOSED OF RX(10), RX(11)  
RX(26) AD ==> AH



AH  
YIELD 90%

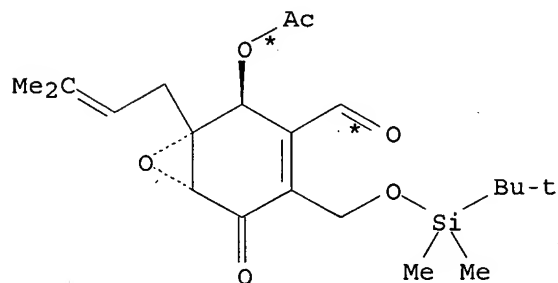
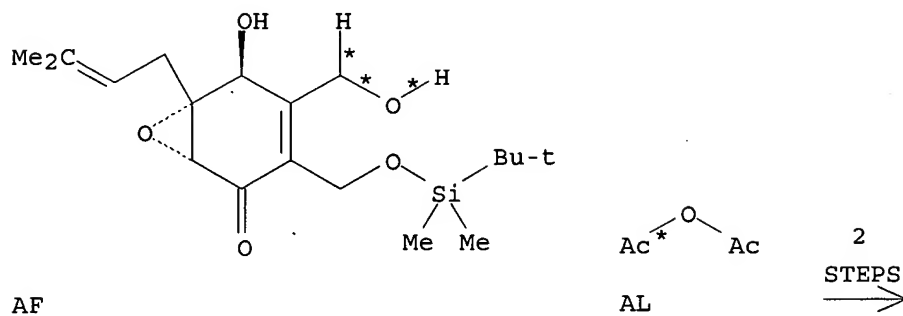
RX(10) RCT AD 674358-47-5  
PRO AF 674358-50-0  
SOL 101-84-8 PhOPh  
CON 6 minutes, 220 deg C  
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me<sub>4</sub>-piperidoxyl, AJ 7782-44-7 O<sub>2</sub>  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

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RX(27) OF 201 COMPOSED OF RX(11), RX(12)  
RX(27) AF + AL ==> AM



AM  
YIELD 98%

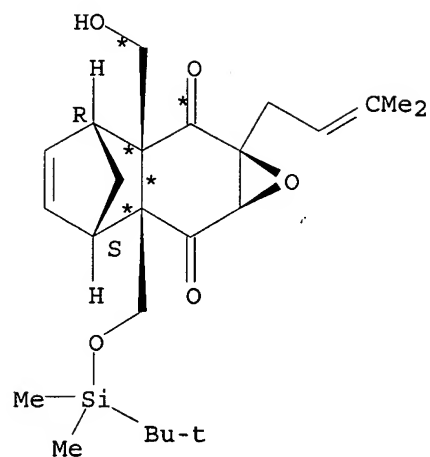
RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

RX(12) RCT AH 674358-53-3, AL 108-24-7  
RGT AN 110-86-1 Pyridine  
PRO AM 674358-56-6  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2  $\text{CH}_2\text{Cl}_2$   
CON 3 hours, 0 deg C

RX(48) OF 201 COMPOSED OF RX(9), RX(10), RX(11)  
RX(48) AC ==> AH

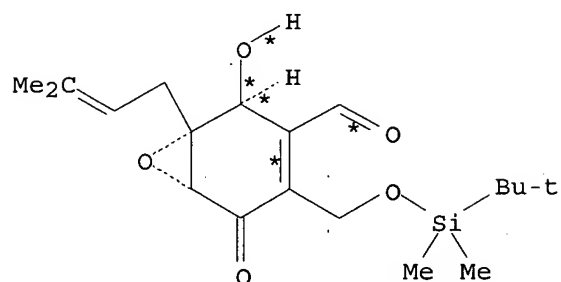
Updated Search

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AC

3  
STEPS  
→



AH

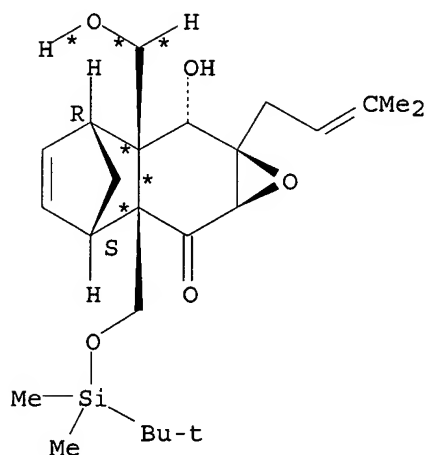
YIELD` 90%

RX(9)	RCT	AC 674358-44-2
	RGT	AE 16940-66-2 NaBH <sub>4</sub>
	PRO	AD 674358-47-5
	SOL	67-56-1 MeOH
	CON	1 hour, -5 deg C
	NTE	regioselective, stereoselective
RX(10)	RCT	AD 674358-47-5
	PRO	AF 674358-50-0
	SOL	101-84-8 PhOPh
	CON	6 minutes, 220 deg C
	NTE	chemoselective, retro-Diels-Alder reaction
RX(11)	RCT	AF 674358-50-0
	RGT	AI 2564-83-2 Me <sub>4</sub> -piperidoxyl, AJ 7782-44-7 O <sub>2</sub>
	PRO	AH 674358-53-3
	CAT	7758-89-6 CuCl
	SOL	68-12-2 DMF
	CON	3 hours, room temperature
	NTE	chemoselective

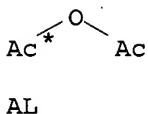
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RX(50) OF 201 COMPOSED OF RX(10), RX(11), RX(12)  
RX(50) AD + AL ==> AM

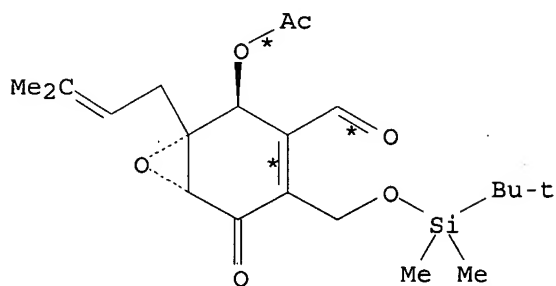


AD



AL

3  
STEPS  
→



AM

YIELD 98%

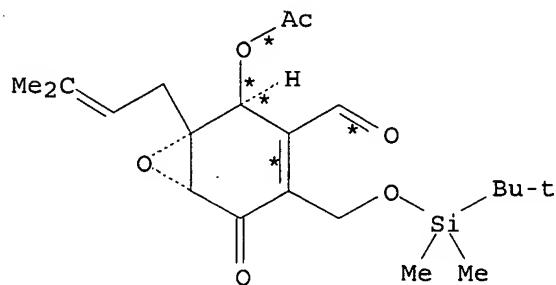
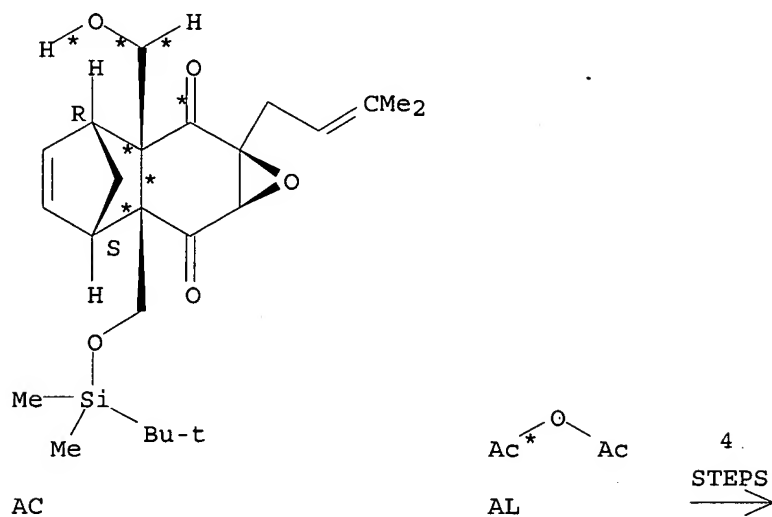
RX(10)	RCT	AD 674358-47-5
	PRO	AF 674358-50-0
	SOL	101-84-8 PhOPh
	CON	6 minutes, 220 deg C
	NTE	chemoselective, retro-Diels-Alder reaction
RX(11)	RCT	AF 674358-50-0
	RGT	AI 2564-83-2 Me <sub>4</sub> -piperidoxyl, AJ 7782-44-7 O <sub>2</sub>
	PRO	AH 674358-53-3
	CAT	7758-89-6 CuCl
	SOL	68-12-2 DMF
	CON	3 hours, room temperature
	NTE	chemoselective
RX(12)	RCT	AH 674358-53-3, AL 108-24-7
	RGT	AN 110-86-1 Pyridine
	PRO	AM 674358-56-6

Updated Search

10509228

CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 3 hours, 0 deg C

RX(51) OF 201 COMPOSED OF RX(9), RX(10), RX(11), RX(12)  
RX(51) AC + AL ==> AM



YIELD 98%

RX(9) RCT AC 674358-44-2  
RGT AE 16940-66-2 NaBH<sub>4</sub>  
PRO AD 674358-47-5  
SOL 67-56-1 MeOH  
CON 1 hour, -5 deg C  
NTE regioselective, stereoselective

RX(10) RCT AD 674358-47-5  
PRO AF 674358-50-0  
SOL 101-84-8 PhOPh  
CON 6 minutes, 220 deg C  
NTE chemoselective, retro-Diels-Alder reaction

Updated Search



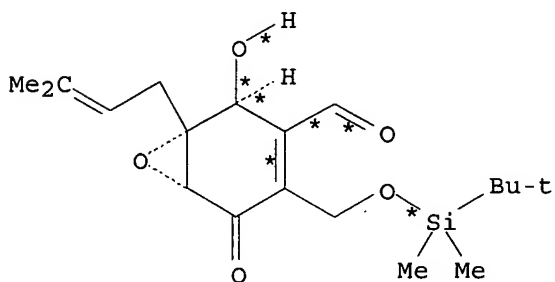
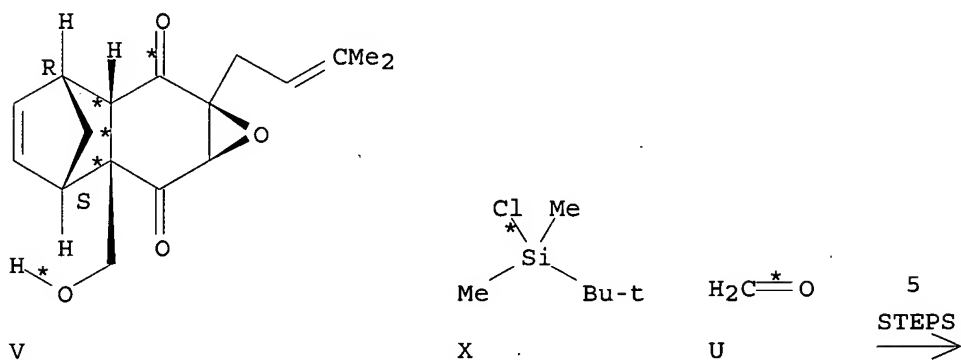
10509228

RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

RX(12) RCT AH 674358-53-3, AL 108-24-7  
RGT AN 110-86-1 Pyridine  
PRO AM 674358-56-6  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON 3 hours, 0 deg C

RX(83) OF 201 COMPOSED OF RX(7), RX(8), RX(9), RX(10), RX(11)

RX(83) V + X + U ==> AH



AH  
YIELD 90%

RX(7) RCT V 674358-38-4, X 18162-48-6  
RGT Z 1122-58-3 4-DMAP, AA 288-32-4 1H-Imidazole  
PRO Y 674358-41-9  
SOL 68-12-2 DMF  
CON 0 deg C

RX(8) RCT Y 674358-41-9, U 50-00-0

Updated Search

10509228

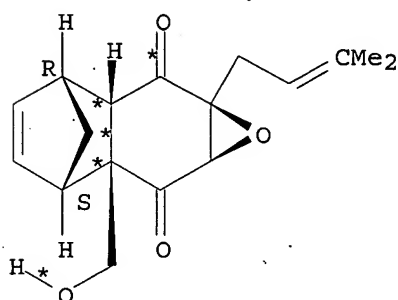
RGT W 6674-22-2 DBU  
PRO AC 674358-44-2  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 36 hours, 0 deg C

RX(9) RCT AC 674358-44-2  
RGT AE 16940-66-2 NaBH4  
PRO AD 674358-47-5  
SOL 67-56-1 MeOH  
CON 1 hour, -5 deg C  
NTE regioselective, stereoselective

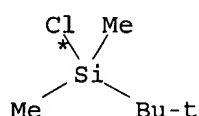
RX(10) RCT AD 674358-47-5  
PRO AF 674358-50-0  
SOL 101-84-8 PhOPh  
CON 6 minutes, 220 deg C  
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

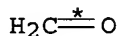
RX(88) OF 201 COMPOSED OF RX(7), RX(8), RX(9), RX(10), RX(11), RX(12)  
RX(88) V + X + U + AL ==> AM



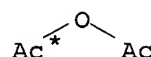
V



X



U

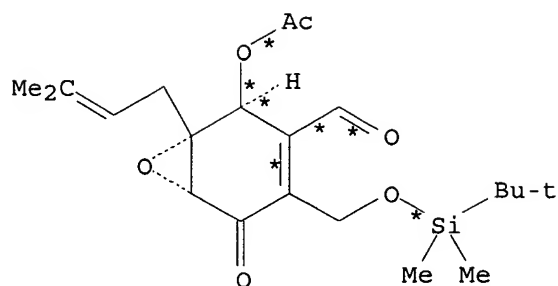


AL

6  
STEPS  
→

Updated Search

10509228



AM  
YIELD 98%

RX(7) RCT V 674358-38-4, X 18162-48-6  
RGT Z 1122-58-3 4-DMAP, AA 288-32-4 1H-Imidazole  
PRO Y 674358-41-9  
SOL 68-12-2 DMF  
CON 0 deg C

RX(8) RCT Y 674358-41-9, U 50-00-0  
RGT W 6674-22-2 DBU  
PRO AC 674358-44-2  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 36 hours, 0 deg C

RX(9) RCT AC 674358-44-2  
RGT AE 16940-66-2 NaBH<sub>4</sub>  
PRO AD 674358-47-5  
SOL 67-56-1 MeOH  
CON 1 hour, -5 deg C  
NTE regioselective, stereoselective

RX(10) RCT AD 674358-47-5  
PRO AF 674358-50-0  
SOL 101-84-8 PhOPh  
CON 6 minutes, 220 deg C  
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me<sub>4</sub>-piperidoxyl, AJ 7782-44-7 O<sub>2</sub>  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

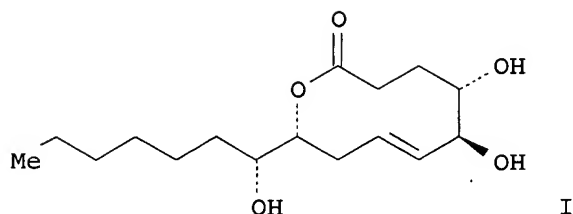
RX(12) RCT AH 674358-53-3, AL 108-24-7  
RGT AN 110-86-1 Pyridine  
PRO AM 674358-56-6  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 3 hours, 0 deg C

L3 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 140:199131 CASREACT

Updated Search

10509228

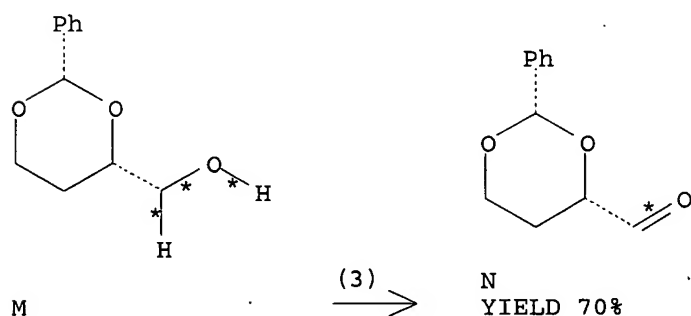
TITLE: Stereoselective total synthesis of the nonenolide  
(+)-microcarpalide  
AUTHOR(S): Banwell, Martin G.; Loong, David T. J.  
CORPORATE SOURCE: Research School of Chemistry, Institute of Advanced  
Studies, The Australian National University, Canberra,  
ACT 0200, Australia  
SOURCE: Heterocycles (2004), 62, 713-734  
CODEN: HTCYAM; ISSN: 0385-5414  
PUBLISHER: Japan Institute of Heterocyclic Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The enantiomer, (+)-microcarpalide (I), of the nonenolide natural product  
(+)-microcarpalide has been prepared from (S)-malic acid and 3-decyn-1-ol  
via a sixteen step sequence involving ring closing metathesis (RCM).

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 288 ...M ==> N...



RX(3) RCT M 103773-79-1

STAGE(1)

RGT O 3240-34-4 PhI(OAc)<sub>2</sub>, P 14691-89-5  
1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 14 hours, 18 deg C

STAGE(2)

RGT E 144-55-8 NaHCO<sub>3</sub>

Updated Search

10509228

SOL 7732-18-5 Water  
CON 18 deg C

PRO N 145958-02-7

L3 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:111158 CASREACT

TITLE: Milbemycin  $\alpha$ 17 and related compounds synthesized from milbemycin A4: Synthetic procedure and acaricidal activities

AUTHOR(S): Tsukiyama, Takahiro; Kinoshita, Ayakoe; Ichinose, Reiji; Sato, Kazuo

CORPORATE SOURCE: Agrosience Research Laboratories, Sankyo Agro Co., Ltd., Shiga, 520-2342, Japan

SOURCE: Journal of Antibiotics (2003), 56(10), 848-855  
CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

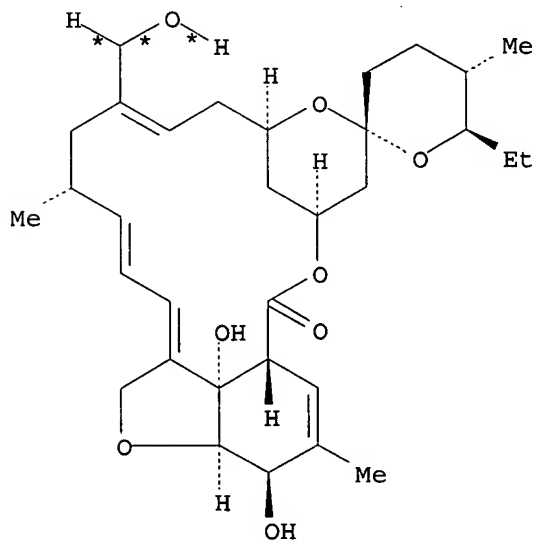
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Milbemycin  $\alpha$ 17 (I), a 14-demethyl congener of milbemycin A4, has been reported as a natural product. In this paper, we report the successful development of a chemical derivation method to synthesize milbemycin  $\alpha$ 17 from milbemycin A4, as well as our use of a similar method to prepare 24-demethylmilbemycin A4' from the same precursor. Thus, I was prepared by desilylation of the 5-O-TBDMS ether which was prepared by decarbonylation of 5-O-TBDMS-14-formylmilbemycin A4. The acaricidal activities of these compds. were assessed against the organophosphorus-sensitive two-spotted spider mites (*Tetranychus urticae*) on the primary leaves of cowpea plants (*Vigna sinensis* Savi species) by spraying.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 28 ...K ==> M...

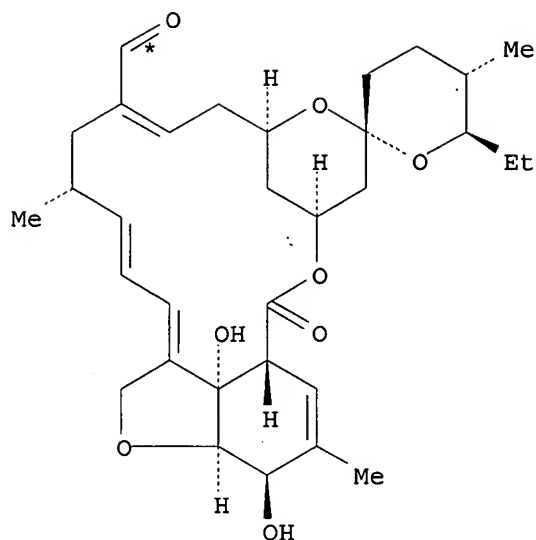


K

(5) →

Updated Search

10509228



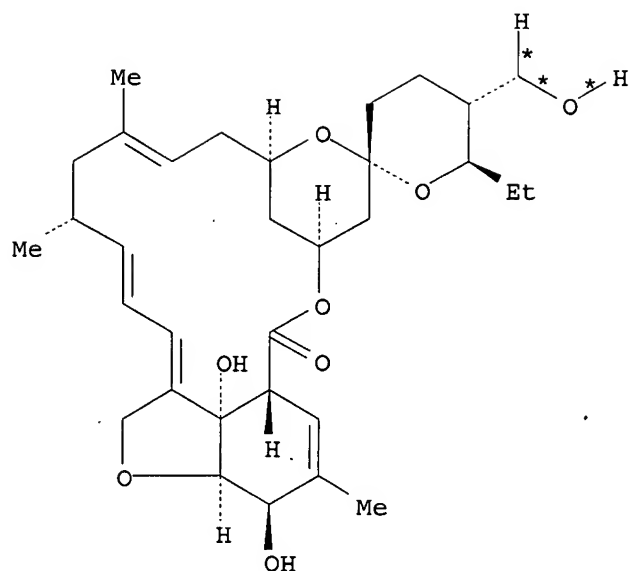
M  
YIELD 87%

RX(5) RCT K 112774-81-9  
RGT N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NCl, R 128-09-6  
Chlorosuccinimide  
PRO M 112774-92-2  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature  
NTE regioselective

RX(9) OF 28 AB ==> AC...

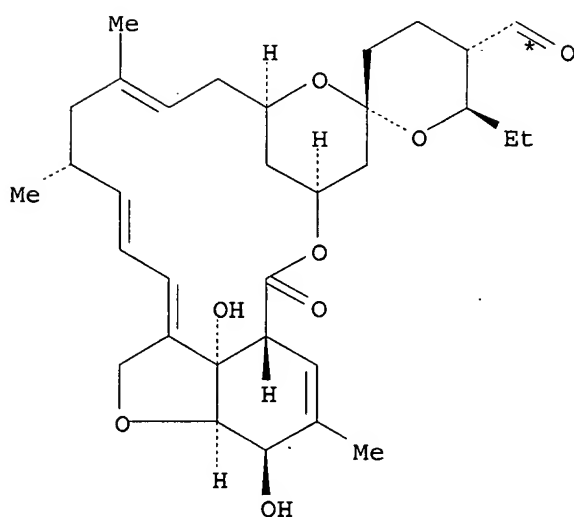
Updated Search

10509228



AB

(9)



AC

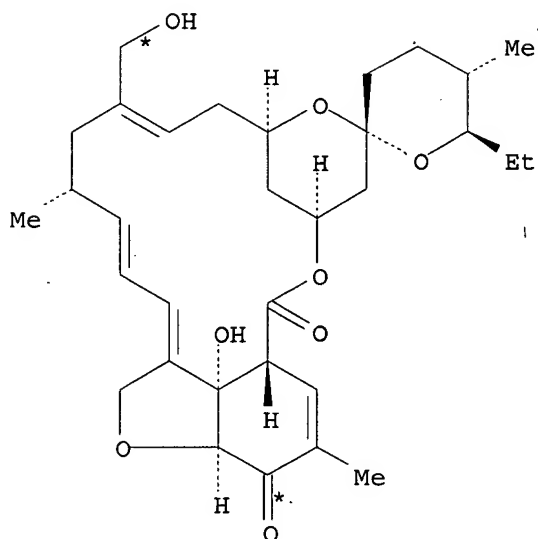
YIELD 53%

RX(9)      RCT    AB 123022-52-6  
 RGT    N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
          Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NCl, R 128-09-6  
          Chlorosuccinimide  
 PRO    AC 482621-67-0  
 SOL    7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON    1 hour, room temperature  
 NTE    regioselective

Updated Search

10509228

RX(13) OF 28 COMPOSED OF RX(4), RX(5)  
RX(13) G ==> M



2  
STEPS  
→

G

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT G 141547-92-4  
RGT L 16940-66-2 NaBH4  
PRO K 112774-81-9  
SOL 67-56-1 MeOH  
CON 10 minutes, 0 deg C  
NTE stereoselective

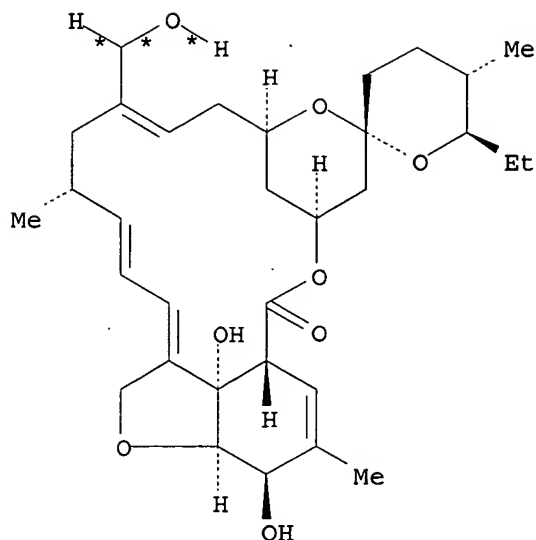
RX(5) RCT K 112774-81-9  
RGT N 144-55-8 NaHCO3, O 584-08-7 K2CO3, P 2564-83-2  
Me4-piperidoxyl, Q 1112-67-0 Bu4NCl, R 128-09-6  
Chlorosuccinimide  
PRO M 112774-92-2  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 1 hour, room temperature  
NTE regioselective

RX(14) OF 28 COMPOSED OF RX(5), RX(6)  
RX(14) K + T ==> U

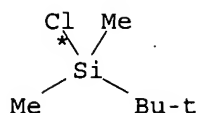
Updated Search



10509228



K



T

2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

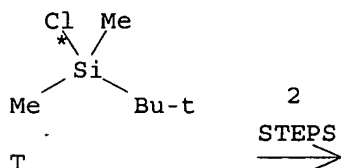
RX(5) RCT K 112774-81-9  
RGT N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NCl, R 128-09-6  
Chlorosuccinimide  
PRO M 112774-92-2  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature  
NTE regioselective

RX(6) RCT M 112774-92-2, T 18162-48-6  
RGT V 288-32-4 1H-Imidazole  
PRO U 112774-91-1  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

RX(17) OF 28 COMPOSED OF RX(9), RX(10)

RX(17) AB + T ==> AD

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



T

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

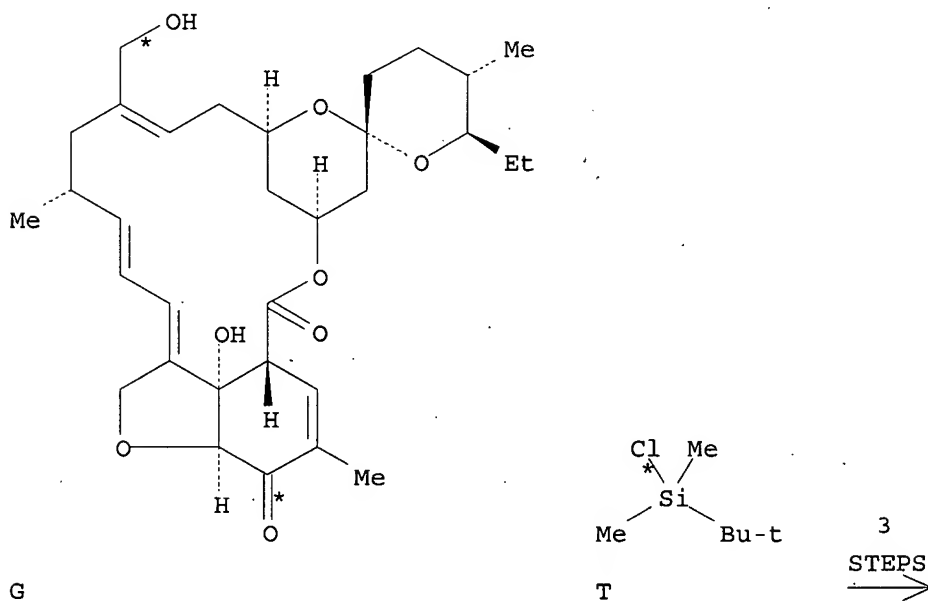
Updated Search

10509228

RX(9) RCT AB 123022-52-6  
RGT N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NC<sub>1</sub>, R 128-09-6  
Chlorosuccinimide  
PRO AC 482621-67-0  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature  
NTE regioselective

RX(10) RCT AC 482621-67-0, T 18162-48-6  
RGT V 288-32-4 1H-Imidazole  
PRO AD 482621-71-6  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

RX(20) OF 28 COMPOSED OF RX(4), RX(5), RX(6)  
RX(20) G + T ==> U



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT G 141547-92-4  
RGT L 16940-66-2 NaBH<sub>4</sub>  
PRO K 112774-81-9  
SOL 67-56-1 MeOH  
CON 10 minutes, 0 deg C  
NTE stereoselective

RX(5) RCT K 112774-81-9  
RGT N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NC<sub>1</sub>, R 128-09-6  
Chlorosuccinimide  
PRO M 112774-92-2

Updated Search

10509228

SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature  
NTE regioselective

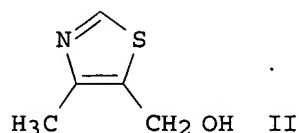
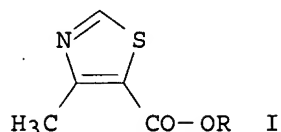
RX(6) RCT M 112774-92-2, T 18162-48-6  
RGT V 288-32-4 1H-Imidazole  
PRO U 112774-91-1  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

L3 ANSWER 23 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 139:337963 CASREACT  
TITLE: Oxidation and reduction process for the preparation of  
5-formyl-4-methylthiazole  
INVENTOR(S): Deshpande, Pandurang Balwant; Luthra, Parven Kumar;  
Vyas, Rajesh; Kamma, Ramakrishna  
PATENT ASSIGNEE(S): Orchid Chemicals & Pharmaceuticals Limited, India  
SOURCE: U.S. Pat. Appl. Publ., 4 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003204095	A1	20031030	US 2002-309812	20021205
US 6833459	B2	20041221		
IN 194928	A	20041211	IN 2002-MA325	20020426
CA 2483482	AA	20031106	CA 2002-2483482	20021210
WO 2003091230	A1	20031106	WO 2002-IB5270	20021210
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002367890	A1	20031110	AU 2002-367890	20021210
CN 1628108	A	20050615	CN 2002-829187	20021210
JP 2005526112	T2	20050902	JP 2003-587790	20021210
PRIORITY APPLN. INFO.:			IN 2002-MA325	20020426
			WO 2002-IB5270	20021210
OTHER SOURCE(S):	MARPAT 139:337963			
GI				

Updated Search

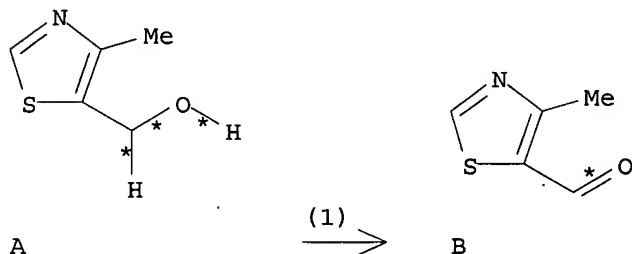
10509228



AB 4-Methyl-5-formylthiazole is prepd in high yield and selectivity by the reduction of the corresponding ester (I; R = C1-4 alkyl; e.g., Et 4-methyl-5-thiazolecarboxylate) into 5-(hydroxymethyl)-4-methylthiazole (II) which is then subjected to liquid-phase oxidation to give the product aldehyde.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 5 ...A ==> B



RX(1) RCT A 1977-06-6

STAGE(1)

SOL 75-09-2 CH2Cl2  
CON 5 minutes, room temperature

STAGE(2)

RGT C 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 30 - 32 deg C  
SUBSTAGE(2) 5 - 10 minutes, 30 - 32 deg C

STAGE(3)

RGT D 7758-02-3 KBr, E 2564-83-2 Me4-piperidoxyl, F  
7681-52-9 NaOCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 32 deg C -> 0 deg C

Updated Search

10509228

SUBSTAGE(3) 1 hour, 0 - 2 deg C  
SUBSTAGE(4) 0 - 2 deg C

PRO B 82294-70-0

L3 ANSWER 24 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 138:24587 CASREACT

TITLE: Process for the preparation of prostaglandins and analogs

INVENTOR(S): Greenwood, Alan Kenneth; McHattie, Derek; Thompson, David George; Clissold, Derek Wyndham

PATENT ASSIGNEE(S): Resolution Chemicals Limited, UK; Cascade Biochem Limited

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

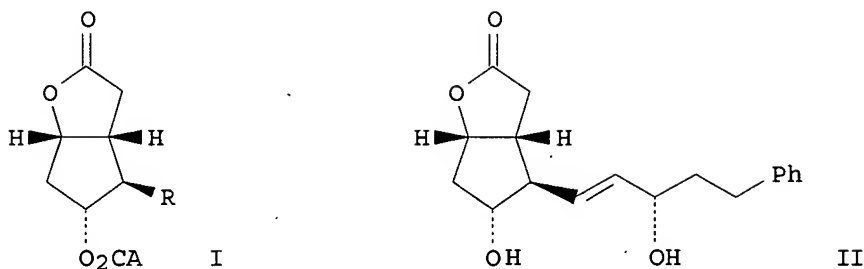
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096898	A2	20021205	WO 2002-GB2462	20020524
WO 2002096898	A3	20030320		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2448088	AA	20021205	CA 2002-2448088	20020524
NZ 529634	A	20031219	NZ 2002-529634	20020524
EP 1389198	A2	20040218	EP 2002-755096	20020524
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2002009984	A	20040406	BR 2002-9984	20020524
CN 1533385	A	20040929	CN 2002-814634	20020524
JP 2005503354	T2	20050203	JP 2003-500077	20020524
US 2004249172	A1	20041209	US 2004-478513	20040608
US 2005261374	A1	20051124	US 2005-189985	20050727
US 2005272877	A1	20051208	US 2005-189986	20050727
PRIORITY APPLN. INFO.:			GB 2001-12699	20010524
			WO 2002-GB2462	20020524
			US 2004-478513	20040608

OTHER SOURCE(S): MARPAT 138:24587

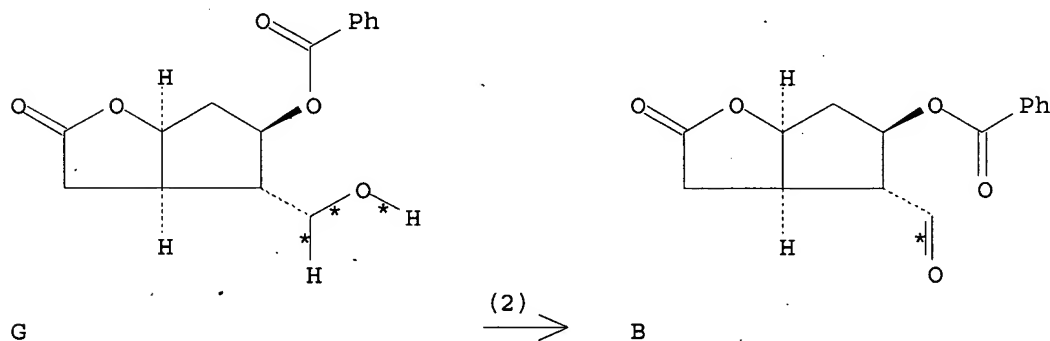
GI

10509228



AB The formylloxabicyclooctanones I (A = C6-10-aryl which may be substituted by halo, alkyl, aryl) were prepared by oxidation of the corresponding alcs. as intermediates for prostaglandin synthesis especially analogs of PGF2 $\alpha$ . Thus, (-)-benzyl Corey lactone (I, R = CH2OH, A = Ph) was treated with NaOCl, TEMPO and KBr in CH2Cl2 to give I (R = CHO, A = Ph), which was converted to latanoprost in several steps by standard methods, via derivative II.

RX(2) OF 66      G ==> B...



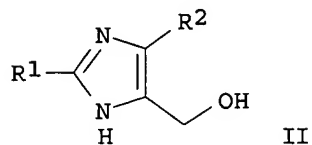
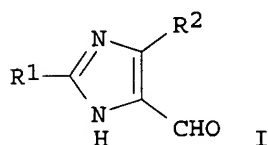
RX(2)      RCT    G 39746-00-4  
 RGT    H 7681-52-9 NaOCl, I 2564-83-2 Me4-piperidoxyl, J  
          7758-02-3 KBr  
 PRO    B 39746-01-5  
 SOL    75-09-2 CH2Cl2

L3    ANSWER 25 OF 38    CASREACT    COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER:      137:247693    CASREACT  
 TITLE:                    Preparation of 4-formylimidazoles  
 INVENTOR(S):            Isokawa, Sorou; Enomoto, Katashi; Nagai, Naoshi  
 PATENT ASSIGNEE(S):    Mitsui Chemicals Inc., Japan  
 SOURCE:                  Jpn. Kokai Tokkyo Koho, 4 pp.  
                              CODEN: JKXXAF  
 DOCUMENT TYPE:        Patent  
 LANGUAGE:               Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

Updated Search

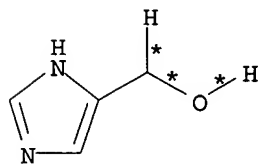
10509228

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275162	A2	20020925	JP 2001-73700	20010315
PRIORITY APPLN. INFO.:			JP 2001-73700	20010315
OTHER SOURCE(S):			MARPAT 137:247693	
GI				



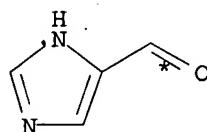
AB The compds. I [R1, R2 = H, C1-10 (un)substituted alkyl, aryl, halo] are prepared by reaction of imidazoles II (R1, R2 = same as I) in the presence of 2,2,6,6-tetramethylpiperidine N-oxyls and cooxidizing agents in organic solvents or water solvents under basic condition.

RX(1) OF 3 A ==> B



● HCl

A



B  
YIELD 57%

RX(1) RCT A 32673-41-9

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,  
4-hydroxy-2,2,6,6-tetramethyl-  
SOL 75-09-2 CH2Cl2

STAGE(2)

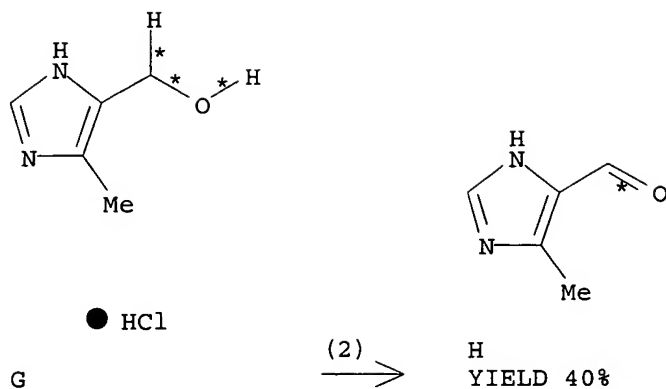
RGT D 7681-52-9 NaOCl  
SOL 7732-18-5 Water

PRO B 3034-50-2

RX(2) OF 3 G ==> H

Updated Search

10509228



RX(2) RCT G 38585-62-5

STAGE(1)

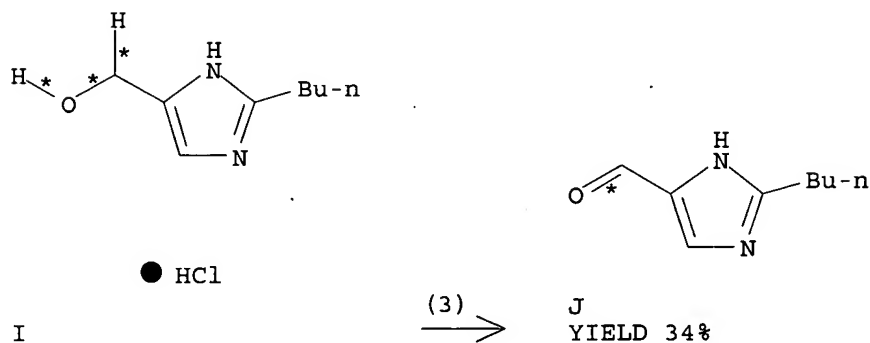
RGT C 2226-96-2 1-Piperidinyloxy,  
4-hydroxy-2,2,6,6-tetramethyl-  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT D 7681-52-9 NaOCl  
SOL 7732-18-5 Water

PRO H 68282-53-1

RX(3) OF 3 I ==> J



RX(3) RCT I 460717-19-5

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,  
4-hydroxy-2,2,6,6-tetramethyl-  
CAT 71-91-0 Et<sub>4</sub>N.Br  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT D 7681-52-9 NaOCl  
SOL 7732-18-5 Water

Updated Search



10509228

PRO J 68282-49-5

L3 ANSWER 26 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 137:201293 CASREACT  
TITLE: Method of synthesizing camptothecin-relating compounds  
INVENTOR(S): Ogawa, Takanori; Nishiyama, Hiroyuki; Uchida, Miyuki;  
Sawada, Seigo  
PATENT ASSIGNEE(S): Kabushiki Kaisha Yakult Honsha, Japan  
SOURCE: PCT Int. Appl., 89 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066416	A1	20020829	WO 2002-JP1538	20020221
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2437702	AA	20020829	CA 2002-2437702	20020221
EE 200300373	A	20031015	EE 2003-373	20020221
EP 1378505	A1	20040107	EP 2002-703874	20020221
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
CN 1492851	A	20040428	CN 2002-805323	20020221
NZ 527615	A	20041224	NZ 2002-527615	20020221
BG 108031	A	20050430	BG 2003-108031	20030725
ZA 2003006223	A	20040603	ZA 2003-6223	20030812
NO 2003003579	A	20031010	NO 2003-3579	20030813
NZ 534374	A	20041224	NZ 2003-534374	20030814
US 2004106830	A1	20040603	US 2003-467987	20031218
PRIORITY APPLN. INFO.:			JP 2001-45430	20010221
			JP 2001-309322	20011005
			JP 2001-309332	20011005
			WO 2002-JP1538	20020221
OTHER SOURCE(S):	MARPAT 137:201293			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

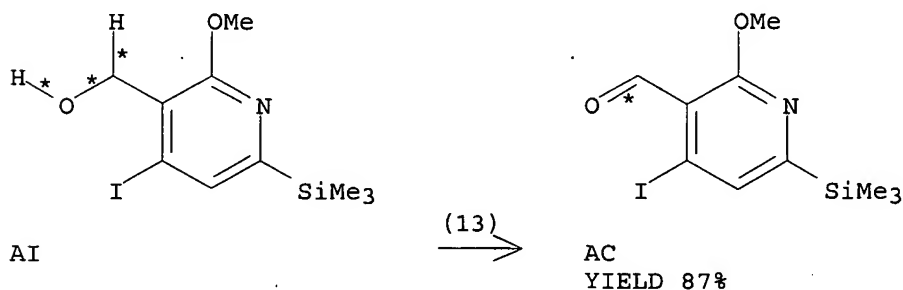
AB 2'-Amino-5'-hydroxypropiophenone (I) corresponding to the AB cycle moiety of the camptothecin (CPT) skeleton and a tricyclic ketone, namely (S)-4-ethyl-7,8-dihydro-4-hydroxy-1H-pyrano[3,4-f]indolizine-3,6,10(4H)-trione (II) corresponding to the CDE cycle moiety thereof can be efficiently produced and thus CPT and its derivs. can be stably supplied by a practically usable total synthesis to more efficiently provide

Updated Search

camptothecin (CPT), which is a starting compound for irinotecan hydrochloride, namely 7-ethyl-10-[4-(1-piperidino)-1-piperidino]carbonyloxycamptothecin hydrochloride trihydrate, and various camptothecin derivs. Thus, benzylation of 2-nitro-5-hydroxybenzaldehyde by benzyl chloride in the presence of K<sub>2</sub>CO<sub>3</sub> in DMF at 60° for 20 h gave 94% 5-benzyloxy-2-nitrobenzaldehyde which went addition reaction with vinylmagnesium bromide in THF at 3-10° for 1 h to give 84.0% 1-(5-benzyloxy-2-nitrophenyl)-2-propen-1-ol (VIII). Oxidation of VIII with MnO<sub>2</sub> in CHCl<sub>3</sub> at 25° for 15 h gave 91% 1-(5-benzyloxy-2-nitrophenyl)-1-oxo-2-propene which was hydrogenated over 10% Pd-C in EtOAc under H atmospheric for 13 h to give 81% I. K<sub>2</sub>OsO<sub>4</sub>·2H<sub>2</sub>O and (DHQD)2Pyr were added to an aqueous solution of K<sub>3</sub>Fe(CN)<sub>6</sub>, K<sub>2</sub>CO<sub>3</sub>, and MeSO<sub>2</sub>NH<sub>2</sub> and stirred at .apprx.5° for 1 h, followed by adding 4-ethyl-8-methoxy-6-(trimethylsilyl)-1H-pyrano[3,4-c]pyridine, and the resulting mixture was stirred at 5° for 20 h, treated with sodium sulfite, and stirred at 5° for 30 min for asym. dihydroxylation to give a diol (III) (95%) which was oxidized by iodine and K<sub>2</sub>CO<sub>3</sub> in aqueous methanol at 40° for 48 h to give a lactone (IV; R = TMS) (88%). Iodination of IV (R = TMS) by iodine and CF<sub>3</sub>CO<sub>2</sub>Ag in CH<sub>2</sub>Cl<sub>2</sub> at room temperature for 16.5 h gave IV (R = iodo) (97%) which underwent carbonylation by CO in the presence of Pd(OAc)<sub>2</sub> and K<sub>2</sub>CO<sub>3</sub> in 1-propanol at 60° for 18 to give an ester IV (R = n-PrO<sub>2</sub>C) (70%). Demethylation of IV (R = n-PrO<sub>2</sub>C) by treatment with Me<sub>3</sub>SiCl and NaI in MeCN at room temperature for 3 h gave a keto lactone, namely 4-ethyl-3,4,7,8-tetrahydro-4-hydroxy-3,8-dioxo-1H-pyrano[3,4-c]pyridine-6-carboxylic acid Pr ester (V) (95%) which was cyclocondensed with tert-Bu acrylate in the presence of K<sub>2</sub>CO<sub>3</sub> in DMSO at 50° for 20 min to give a tricyclic compound (VI) (77%). VI was heated with a mixture of CF<sub>3</sub>CO<sub>2</sub>H and PhMe at 110° for 100 min to give 77% II which was cyclocondensed with I in a 1:1 mixture of AcOH and toluene in the presence of p-toluenesulfonic acid monohydrate at 100° for 18 h to give SN-38 (VII; R<sub>1</sub> = H). VII (R<sub>1</sub> = H) was converted into irinotecan hydrochloride, VII.HCl (R<sub>1</sub> = Q).

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(13) OF 249 AI ==> AC



RX(13) RCT AI 375346-05-7  
 RGT AO 7681-52-9 NaOCl, AP 2564-83-2 Me4-piperidoxyl  
 PRO AC 174092-75-2  
 SOL 7732-18-5 Water, 108-88-3 PhMe  
 NTE oxidn. at 0-5° for 2 h

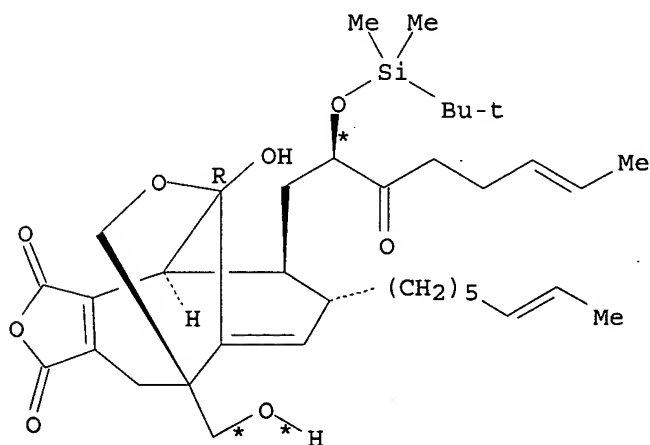
L3 ANSWER 27 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

ACCESSION NUMBER: 136:325339 CASREACT  
TITLE: Total Synthesis of the CP-Molecules (CP-263,114 and CP-225,917, Phomoidrides B and A). 2. Model Studies for the Construction of Key Structural Elements and First-Generation Strategy  
AUTHOR(S): Nicolaou, K. C.; Baran, P. S.; Zhong, Y.-L.; Fong, K. C.; Choi, H.-S.  
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA  
SOURCE: Journal of the American Chemical Society (2002), 124(10), 2190-2201  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Crucial model synthetic and mechanistic studies directed toward the development of methodol. for the construction of the maleic anhydride moiety of the title CP-mols. are described. Studies directed toward the stereoselective attachment of the upper side chain, culminating in the discovery of long-range stereochem. control, are also discussed. In addition, a first-generation strategy toward the CP-mols., establishing a tricyclic diketone key intermediate as a "beachhead" from which all future operations would diverge, is also presented. Although this first-generation strategy failed to yield the target mols., the endeavor laid the important groundwork for the next-generation drives toward the CP-mols.  
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

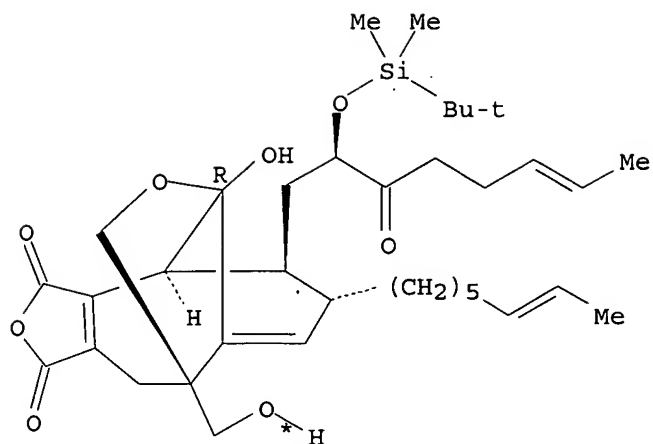
RX(362) OF 443 COMPOSED OF RX(38), RX(39), RX(40), RX(1), RX(43)  
RX(362) 2 I + 2 BX + BA ==> DI



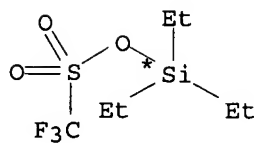
I

Updated Search

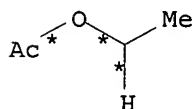
10509228



I

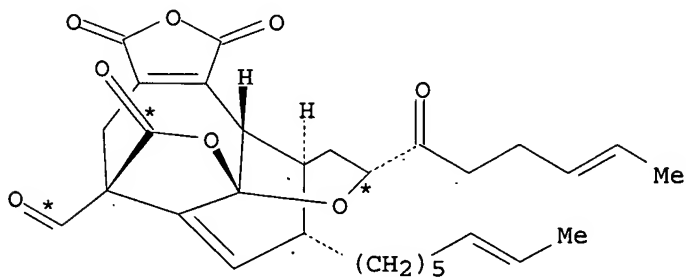


2 BX



BA

5  
STEPS  
→



DI

YIELD 95%

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

Updated Search

10509228

STAGE(1)

RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6  
RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4  
PhI(OAc)2  
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H  
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3  
SOL 75-09-2 CH2Cl2

STAGE(2)

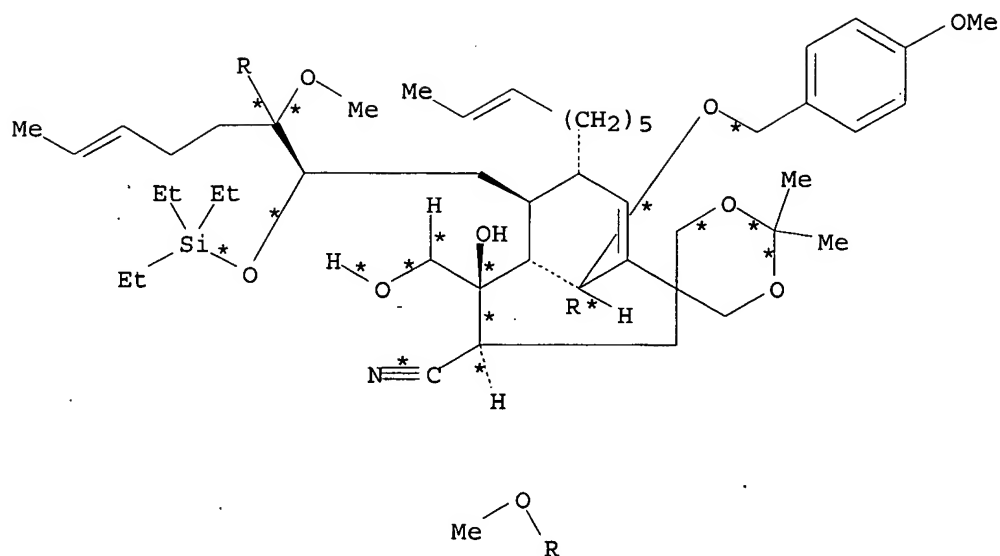
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

RX(367) OF 443 COMPOSED OF RX(28), RX(3), RX(36), RX(37), RX(2), RX(38),  
RX(39), RX(40), RX(1), RX(43)

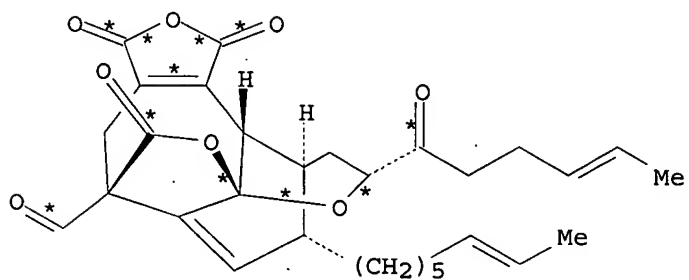
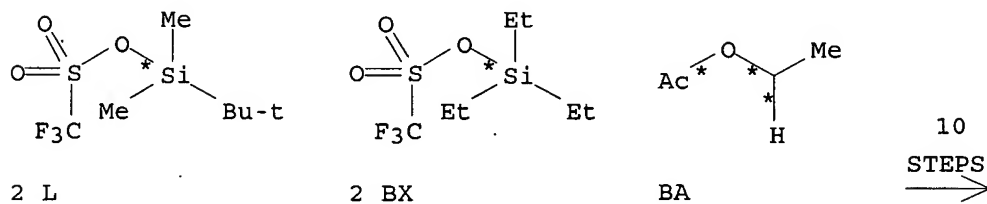
RX(367) 2 CJ + 2 L + 2 BX + BA ==> DI

10509228



CJ

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DI  
YIELD 95%

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO<sub>2</sub>Cl, AC 121-44-8 Et<sub>3</sub>N

Updated Search

10509228

SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K<sub>2</sub>CO<sub>3</sub>

SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O<sub>2</sub>

SOL 60-29-7 Et<sub>2</sub>O

STAGE(4)

RGT AF 144-62-7 (CO<sub>2</sub>H)<sub>2</sub>

PRO K 241819-21-6

NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me<sub>2</sub>C(OMe)<sub>2</sub>

CAT 3144-16-9 10-CSA

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(3)

RCT L 69739-34-0

RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9

RGT BG 20039-37-6 PDC

PRO H 241819-25-0

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(2) RCT H 241819-25-0

PRO I 241819-26-1

SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

Updated Search

10509228

STAGE(1)  
RGT O 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH2Cl2

STAGE(2)  
RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)  
RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)  
RCT BA 141-78-6  
RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)  
RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4  
PhI(OAc)2  
SOL 75-05-8 MeCN

STAGE(2)  
RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)  
RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)  
RGT D 75-75-2 MeSO3H  
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)  
RGT P 144-55-8 NaHCO3  
SOL 75-09-2 CH2Cl2

STAGE(2)  
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8



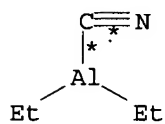
10509228

RX(368) OF 443 COMPOSED OF RX(27), RX(28), RX(3), RX(36), RX(37), RX(2),  
RX(38), RX(39), RX(40), RX(1), RX(43)

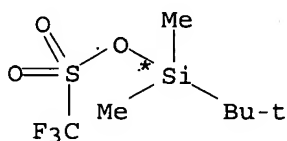
RX(368) 2 CI + 2 AY + 2 L + 2 BX + BA ==> DI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

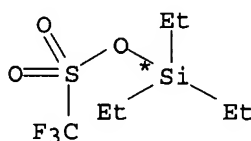
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



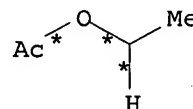
2 AY



2 L

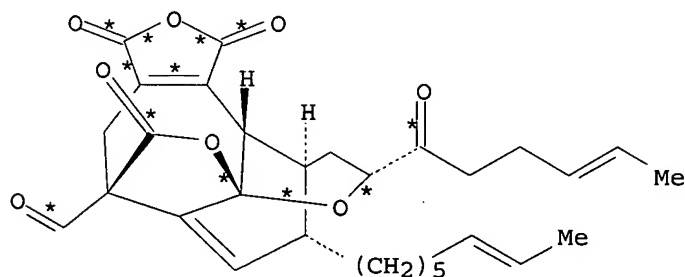


2 BX



BA

11  
STEPS  
→



DI  
YIELD 95%

RX(27) RCT CI 241819-46-5, AY 5804-85-3  
PRO CJ 412943-08-9  
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO2Cl, AC 121-44-8 Et3N  
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K2CO3  
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O2  
SOL 60-29-7 Et2O

STAGE(4)

Updated Search

10509228

RGT AF 144-62-7 (CO<sub>2</sub>H)<sub>2</sub>

PRO K 241819-21-6

NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me<sub>2</sub>C(OMe)<sub>2</sub>

CAT 3144-16-9 10-CSA

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(3)

RCT L 69739-34-0

RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9

RGT BG 20039-37-6 PDC

PRO H 241819-25-0

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(2) RCT H 241819-25-0

PRO I 241819-26-1

SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

Updated Search

10509228

STAGE(1)

RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6  
RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4  
PhI(OAc)2  
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H  
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3  
SOL 75-09-2 CH2Cl2

STAGE(2)

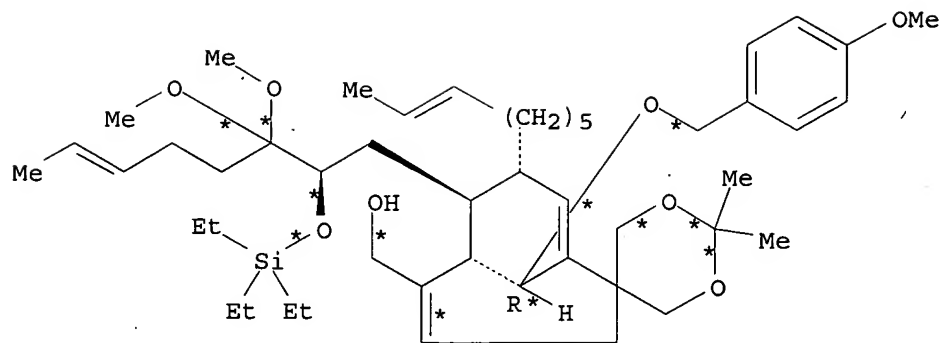
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

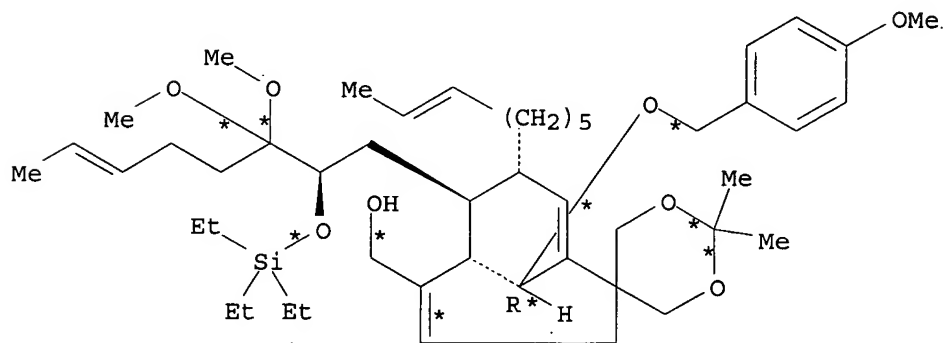
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RX(2), RX(38), RX(39), RX(40), RX(1), RX(43)

RX(369) 2 CH + 2 AY + 2 L + 2 BX + BA ==> DI

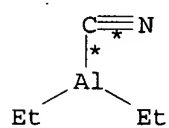
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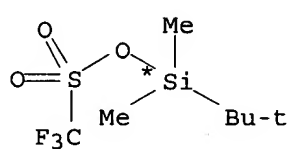
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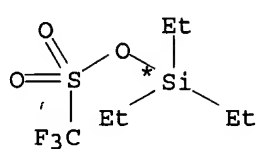
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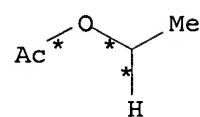
2 AY



2 L

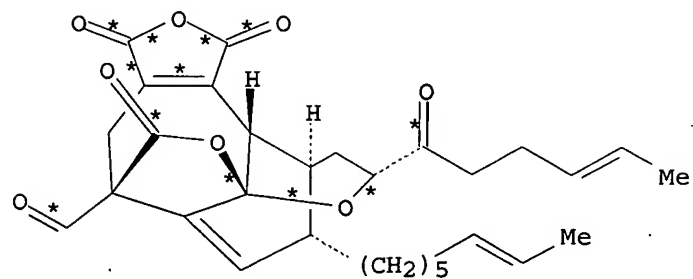


2 BX



BA

12  
STEPS  
→



DI  
YIELD 95%

Updated Search

10509228

RX(26) RCT CH 241819-19-2  
RGT AT 75-91-2 t-BuOOH  
PRO CI 241819-46-5  
CAT 3153-26-2 VO acetylacetonate  
SOL 71-43-2 Benzene, 124-18-5 Decane

RX(27) RCT CI 241819-46-5, AY 5804-85-3  
PRO CJ 412943-08-9  
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO<sub>2</sub>Cl, AC 121-44-8 Et<sub>3</sub>N  
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O<sub>2</sub>  
SOL 60-29-7 Et<sub>2</sub>O

STAGE(4)

RGT AF 144-62-7 (CO<sub>2</sub>H)<sub>2</sub>

PRO K 241819-21-6

NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me<sub>2</sub>C(OMe)<sub>2</sub>  
CAT 3144-16-9 10-CSA  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(3)

RCT L 69739-34-0  
RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO<sub>3</sub>

Updated Search

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SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9  
RGT BG 20039-37-6 PDC  
PRO H 241819-25-0  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(2) RCT H 241819-25-0  
PRO I 241819-26-1  
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6  
RGT P 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me<sub>4</sub>-piperidoxyl, DE 3240-34-4  
PhI(OAc)<sub>2</sub>  
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO<sub>3</sub>H  
SOL 67-66-3 CHCl<sub>3</sub>

Updated Search

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PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3

SOL 75-09-2 CH2Cl2

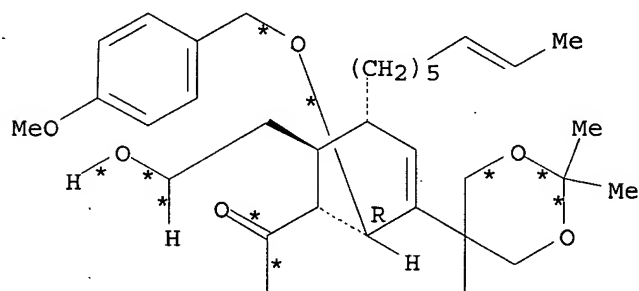
STAGE(2)

RGT BS 87413-09-0 Martin's reagent

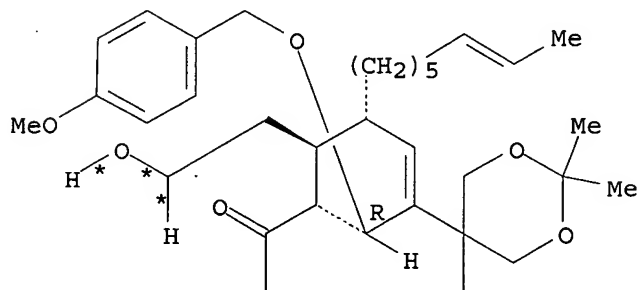
PRO DI 241819-31-8

RX(442) OF 443 COMPOSED OF RX(19), RX(20), RX(21), RX(22), RX(23), RX(24),  
RX(25), RX(26), RX(27), RX(28), RX(3), RX(36), RX(37), RX(2), RX(38),  
RX(39), RX(40), RX(1), RX(43)

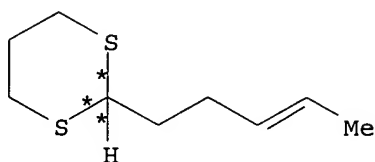
RX(442) 2 BP + 2 BT + 5 BX + S + 3 AI + 2 AG + 2 AY +  
2 L + BA ==> DI



BP



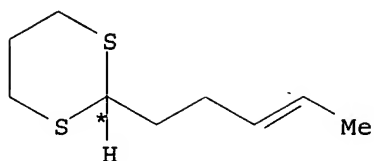
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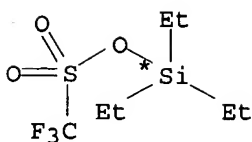
BT

Updated Search

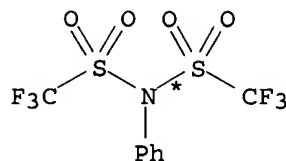
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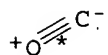
BT



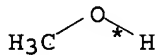
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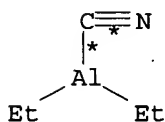
S



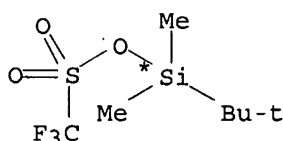
3 AI



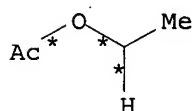
2 AG



2 AY

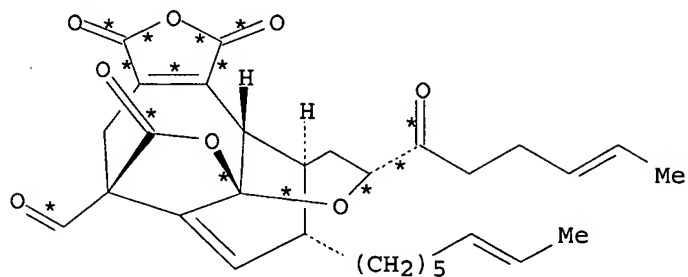


2 L



BA

19  
STEPS  
→



DI

YIELD 95%

RX(19) RCT BP 412943-02-3  
RGT P 144-55-8 NaHCO3, BS 87413-09-0 Martin's reagent  
PRO BR 241819-12-5  
SOL 75-09-2 CH2Cl2

RX(20) RCT BT 241819-10-3

STAGE(1)

RGT BV 109-72-8 BuLi  
SOL 109-99-9 THF, 110-54-3 Hexane

Updated Search



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STAGE(2)

RCT BR 241819-12-5  
SOL 109-99-9 THF

STAGE(3)

RGT AM 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO BU 412943-03-4  
NTE stereoselective

RX(21) RCT BU 412943-03-4

STAGE(1)

RGT CA 7646-69-7. NaH  
SOL 109-99-9 THF

STAGE(2)

RCT BX 79271-56-0  
SOL 109-99-9 THF

STAGE(3)

RGT AM 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO BY 412943-04-5, BZ 412943-32-9

RX(22) RCT BY 412943-04-5, S 37595-74-7  
RGT U 40949-94-8 K [N(SiMe3)2]  
PRO CB 412943-05-6  
SOL 109-99-9 THF, 108-88-3 PhMe

RX(23) RCT AI 630-08-0

STAGE(1)

RGT AL 603-35-0 PPh3  
CAT 3375-31-3 Pd(OAc)2  
SOL 67-56-1 MeOH, 121-44-8 Et3N

STAGE(2)

RCT CB 412943-05-6  
SOL 68-12-2 DMF

STAGE(3)

RGT AM 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO CC 412943-06-7

RX(24) RCT CC 412943-06-7, AG 67-56-1

STAGE(1)

RGT CE 471-34-1 CaCO3, CF 2712-78-9 PhI(O2CCF3)2  
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2, 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

Updated Search

10509228

STAGE(3)

RGT O 108-48-5 2,6-Lutidine, BX 79271-56-0 F3CSO3SiEt3  
SOL 75-09-2 CH2Cl2

STAGE(4)

RGT AG 67-56-1 MeOH

PRO CD 412943-07-8

RX(25) RCT CD 412943-07-8

STAGE(1)

RGT AQ 1191-15-7 AlH(Bu-i)2  
SOL 108-88-3 PhMe

STAGE(2)

RGT AG 67-56-1 MeOH

PRO CH 241819-19-2

RX(26) RCT CH 241819-19-2  
RGT AT 75-91-2 t-BuOOH  
PRO CI 241819-46-5  
CAT 3153-26-2 VO acetylacetonate  
SOL 71-43-2 Benzene, 124-18-5 Decane

RX(27) RCT CI 241819-46-5, AY 5804-85-3  
PRO CJ 412943-08-9  
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO2Cl, AC 121-44-8 Et3N  
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K2CO3  
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O2  
SOL 60-29-7 Et2O

STAGE(4)

RGT AF 144-62-7 (CO2H)2

PRO K 241819-21-6  
NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me2C(OMe)2  
CAT 3144-16-9 10-CSA  
SOL 75-09-2 CH2Cl2

Updated Search

10509228

STAGE(3)

RCT L 69739-34-0  
RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9  
RGT BG 20039-37-6 PDC  
PRO H 241819-25-0  
SOL 75-09-2 CH2Cl2

RX(2) RCT H 241819-25-0  
PRO I 241819-26-1  
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6  
RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

Updated Search

10509228

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4  
Phi(OAc)2  
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H  
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3  
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

L3 ANSWER 28 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 136:5852 CASREACT

TITLE: New process for the preparation of vinyl-pyrrolidinone  
cephalosporin derivatives

INVENTOR(S): Hebeisen, Paul; Hilpert, Hans; Humm, Roland

PATENT ASSIGNEE(S): Basilea Pharmaceutica A.-G., Switz.

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090111	A1	20011129	WO 2001-EP5721	20010518
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002019381	A1	20020214	US 2001-860157	20010517

Updated Search

10509228

US 6504025	B2	20030107		
CA 2408941	AA	20011129	CA 2001-2408941	20010518
EP 1289998	A1	20030312	EP 2001-936374	20010518
EP 1289998	B1	20050330		
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JP 2003535059	T2	20031125	JP 2001-586298	20010518
EP 1435357	A2	20040707	EP 2004-2120	20010518
EP 1435357	A3	20060503		
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CN 1603327	A	20050406	CN 2004-10070031	20010518
AT 292135	E	20050415	AT 2001-936374	20010518
PT 1289998	T	20050630	PT 2001-936374	20010518
ES 2238441	T3	20050901	ES 2001-1936374	20010518

PRIORITY APPLN. INFO.:

EP 2000-111164	20000524
CN 2001-809931	20010518
EP 2001-936374	20010518
WO 2001-EP5721	20010518

OTHER SOURCE(S): MARPAT 136:5852  
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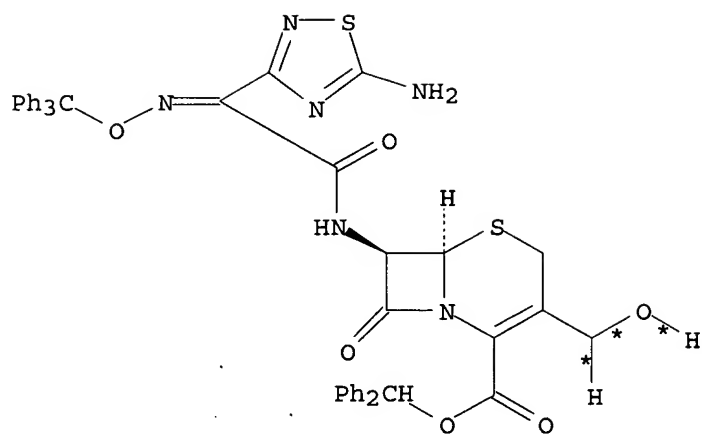
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A process for preparing pharmaceutical compns., a vinyl-pyrrolidinone cephalosporin derivative of I via the acylation of deacetyl-7-aminocephalosporanic acid with II (R1 = a hydroxy protecting group; Y1-Y3 = an activating group) in base followed by the protection of the carboxylic acid group, formation of an aldehyde at C3 using an inorg. hypohalite in TEMPO or with MnO2, and reacting the aldehyde with III (R = an amino protecting group or group A), was accomplished. I can be used for the treatment and prophylaxis of infectious diseases, especially infectious diseases caused by bacterial pathogens in particular methicillin resistant Staphylococcus aureus (MRSA) and Pseudomonas aeruginosa (no data).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

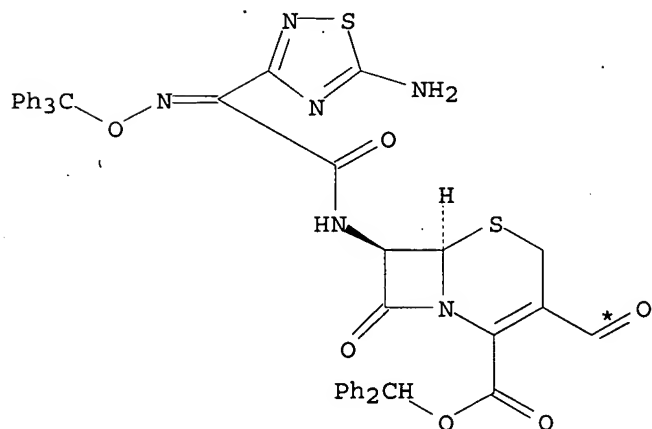
RX(2) OF 29 ...D ==> G...

10509228



D

(2) →



G

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO<sub>3</sub>, J 2564-83-2

Me4-piperidoxyl

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

STAGE(2)

RGT K 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO G 376653-37-1

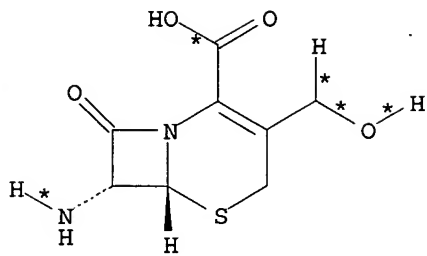
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RX(9) OF 29 COMPOSED OF RX(1), RX(2)

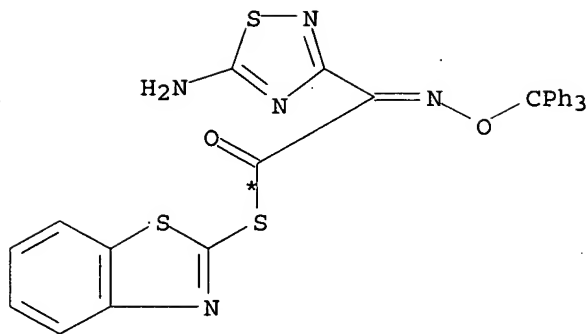
RX(9) A + B + C ==> G

Updated Search

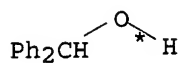
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A

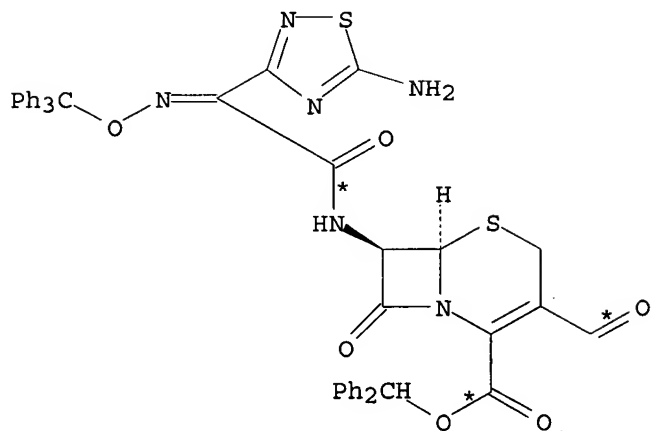


B



C

2  
STEPS  
→



G

RX(1) RCT A 15690-38-7

STAGE(1)

RGT E 80-70-6 Me2NC(:NH)NMe2

SOL 68-12-2 DMF

STAGE(2)

RCT B 209467-59-4, C 91-01-0

PRO D 376653-36-0

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO3, J 2564-83-2

Updated Search

10509228

Me4-piperidoxyl  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT K 7681-52-9 NaOCl  
SOL 7732-18-5 Water

PRO G 376653-37-1  
NTE alternative prepn. shown

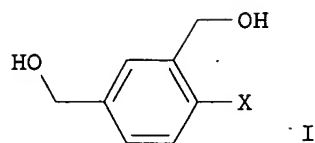
L3 ANSWER 29 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 134:326394 CASREACT  
TITLE: Preparation of citalopram intermediates.  
INVENTOR(S): Ikemoto, Tetsuya; Igi, Masami  
PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan  
SOURCE: Eur. Pat. Appl., 20 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1095926	A2	20010502	EP 2000-118562	20000826
EP 1095926	A3	20030507		
EP 1095926	B1	20041006		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6310222	B1	20011030	US 2000-648048	20000825
AT 278654	E	20041015	AT 2000-118562	20000826
PT 1095926	T	20041231	PT 2000-118562	20000826
ES 2228369	T3	20050416	ES 2000-118562	20000826
CA 2317002	AA	20010501	CA 2000-2317002	20000829
AU 2000055008	A5	20010503	AU 2000-55008	20000830
AU 781464	B2	20050526		
JP 2002121161	A2	20020423	JP 2000-285068	20000920
JP 3641420	B2	20050420		
US 2001056194	A1	20011227	US 2001-909596	20010720
US 6395910	B2	20020528		
US 2002045770	A1	20020418	US 2001-997992	20011130
US 6433195	B2	20020813		
US 2002151728	A1	20021017	US 2002-176721	20020621
US 2004044232	A1	20040304	US 2003-650876	20030828
US 6930211	B2	20050816		
US 2005080278	A1	20050414	US 2003-650875	20030828
US 2006167285	A1	20060727	US 2006-386018	20060321
PRIORITY APPLN. INFO.:			JP 1999-311703	19991101
			JP 2000-245427	20000811
			US 2000-648048	20000825
			US 2001-909596	20010720
			US 2001-997992	20011130
			US 2002-176721	20020621
			US 2003-650875	20030828
OTHER SOURCE(S):	MARPAT 134:326394			
GI				

Updated Search

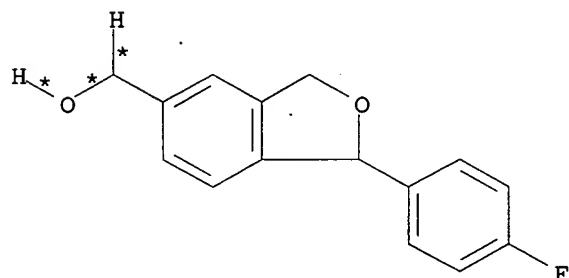


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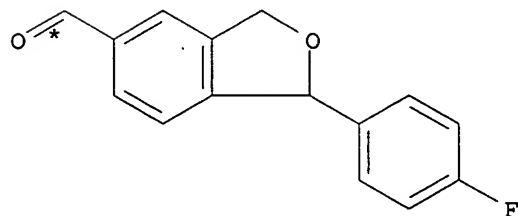


AB Title compds., e.g., (I; X = Cl, Br, iodo), were prepared Thus, 2,4-bis(acetoxymethyl)bromobenzene (preparation given) in MeOH at 10° was treated with aqueous NaOH, stirred for 1 h, and solvent was evaporated The residue was neutralized with aqueous HCl followed by addition of PhMe and heating to 80-85° for 1 h to give 83.7% 2,4-bis(hydroxymethyl)bromobenzene. This was stirred with Et vinyl ether and p-toluenesulfonic acid in PhMe followed by 2 h stirring to give 97.1% 2,4-bis(1-ethoxyethoxymethyl)bromobenzene. The latter in THF at -40° was treated with BuLi followed by warming to -20°, treatment with p-fluorobenzaldehyde, and warming to 15° over 1 h to give 88.7% 1-(4-fluorophenyl)-1,3-dihydrobenzofuran-5-ylmethanol, which was converted to 1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile in 3 steps.

RX(6) OF 28 ...U ==> Z...



U



Z

YIELD 84%

RX(6) RCT U 335612-71-0

Updated Search

## STAGE(1)

RGT AA 144-55-8 NaHCO<sub>3</sub>, AB 1643-19-2 Bu<sub>4</sub>N.Br, AC  
2564-83-2 Me<sub>4</sub>-piperidoxyl  
SOL 141-78-6 AcOEt

## STAGE(2)

RGT AD 7681-52-9 NaOCl  
SOL 7732-18-5 Water

## STAGE(3)

SOL 7732-18-5 Water

PRO Z 335612-72-1

L3 ANSWER 30 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:115518 CASREACT

TITLE: A New Polymer-Attached Reagent for the Oxidation of  
Primary and Secondary Alcohols

AUTHOR(S): Sourkouni-Argirusi, Georgia; Kirschning, Andreas

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet  
Hannover, Hannover, D-30167, Germany

SOURCE: Organic Letters (2000), 2(24), 3781-3784

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

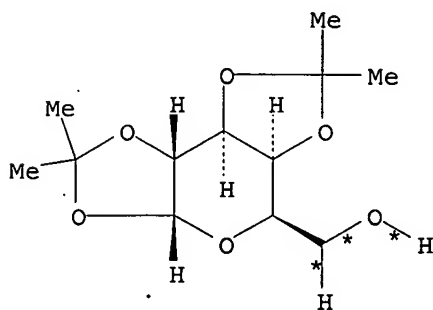
DOCUMENT TYPE: Journal

LANGUAGE: English

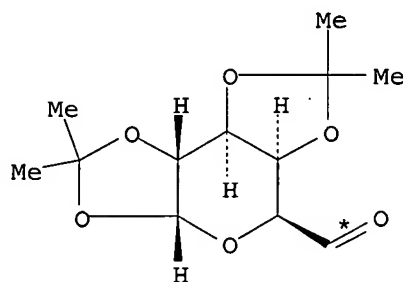
AB A new, polymer-bound reagent system for the efficient oxidation of primary alcs. to aldehydes and secondary alcs. to ketones in the presence of a catalytic amount of 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) is described. The reagent was prepared by treating a com. available polymer-bound bromide (Fluka) with bis(acetato-κO)phenyliodine to give a polymer-bound trimethylammonium-bis(acetato-κO)bromate(1-) reagent. In most cases, workup of this heavy metal-free oxidation is achieved by simple filtration followed by removal of the solvent. In selected examples this reagent was compared with the known polymer-bound permanganate and chromium(VI) reagents.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 18 AC ==> AD



AC

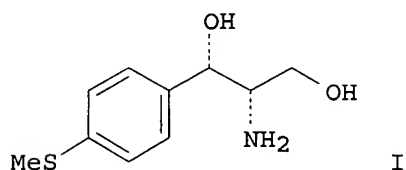


AD  
YIELD 97%

10509228

RX(11) RCT AC 4064-06-6  
RGT D 74-89-5D MeNH<sub>2</sub>, J 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AD 4933-77-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE STEREOSELECTIVE

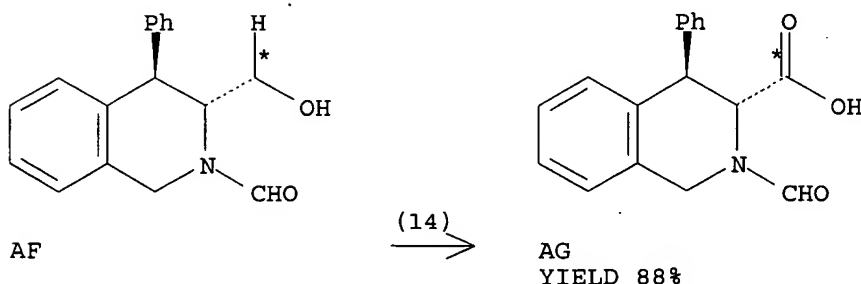
L3 ANSWER 31 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 133:296358 CASREACT  
TITLE: Stereoselective synthesis of 3-mono- and  
1,3-disubstituted 4-phenyl-1,2,3,4-  
tetrahydroisoquinolines  
AUTHOR(S): Brozda, D.; Koroniak, L.; Rozwadowska, M. D.  
CORPORATE SOURCE: Grunwaldzka 6, Faculty of Chemistry, Adam Mickiewicz  
University, Poznan, 60-780, Pol.  
SOURCE: Tetrahedron: Asymmetry (2000), 11(14), 3017-3025  
CODEN: TASYE3; ISSN: 0957-4166  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB (1S,2S)-(+)-Thiomicamine I was transformed in high yield and with high diastereoselectivity into (3R,4R)-4-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid and enantiomerically pure (3R,4R)-3-hydroxymethyl-4-phenyl- and (1R,3R,4R)-3-hydroxymethyl-1-methyl-4-phenyl-1,2,3,4-tetrahydroisoquinoline derivs.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(14) OF 52 ...AF ==> AG...



RX(14) RCT AF 294869-50-4

Updated Search

10509228

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO<sub>3</sub>,  
AJ 7758-02-3 KBr, AK 1112-67-0 Bu<sub>4</sub>NCl  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO<sub>3</sub>, AM 7647-14-5 NaCl  
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

STAGE(5)

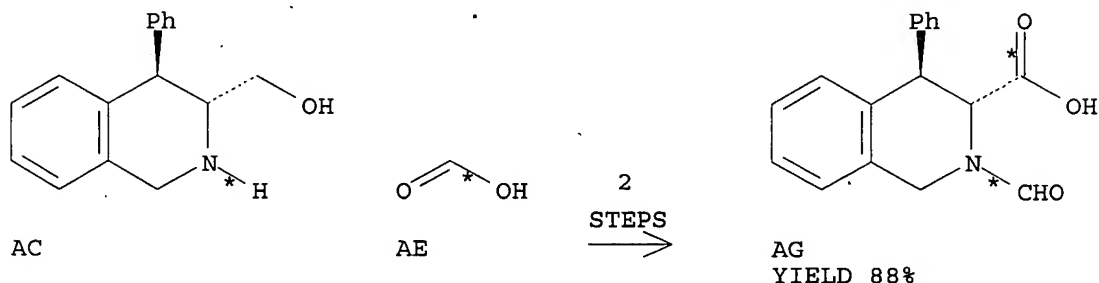
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

PRO AG 294869-51-5

NTE STEREOSELECTIVE

RX(30) OF 52 COMPOSED OF RX(13), RX(14)

RX(30) AC + AE ==> AG



RX(13) RCT AC 300698-53-7, AE 64-18-6

PRO AF 294869-50-4

SOL 108-88-3 PhMe

NTE STEREOSELECTIVE

RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO<sub>3</sub>,  
AJ 7758-02-3 KBr, AK 1112-67-0 Bu<sub>4</sub>NCl  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO<sub>3</sub>, AM 7647-14-5 NaCl  
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

Updated Search

10509228

STAGE(5)

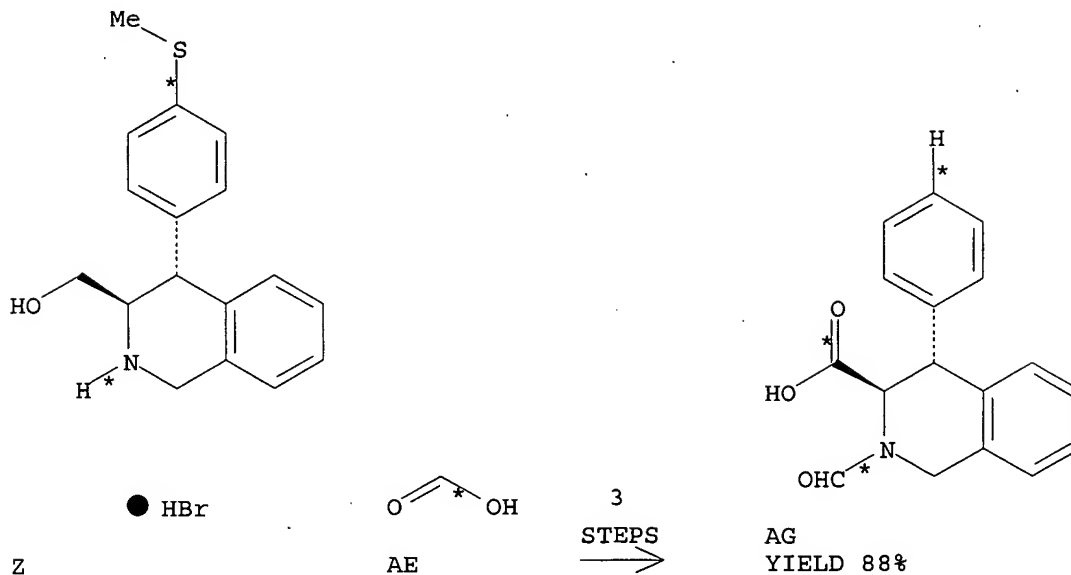
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

PRO AG 294869-51-5

NTE STEREOSELECTIVE

RX(42) OF 52 COMPOSED OF RX(11), RX(13), RX(14)

RX(42) Z + AE ==> AG



RX(11) RCT Z 294869-46-8

STAGE(1)

RGT P 7647-01-0 HCl

SOL 109-99-9 THF

STAGE(2)

RGT AD 7440-02-0 Ni

PRO AC 300698-53-7

NTE STEREOSELECTIVE

RX(13) RCT AC 300698-53-7, AE 64-18-6

PRO AF 294869-50-4

SOL 108-88-3 PhMe

NTE STEREOSELECTIVE

RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me<sub>4</sub>-piperidoxyl, AI 144-55-8 NaHCO<sub>3</sub>,

AJ 7758-02-3 KBr, AK 1112-67-0 Bu<sub>4</sub>NCl

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

Updated Search

10509228

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO<sub>3</sub>, AM 7647-14-5 NaCl  
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

STAGE(5)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

PRO AG 294869-51-5  
NTE STEREOSELECTIVE

L3 ANSWER 32 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 127:65794 CASREACT

TITLE: Oxidation of primary or secondary alcohols using  
N-chloro compounds and piperidinyloxy derivatives.

INVENTOR(S): Jenny, Christian-Johannes; Lohri, Bruno; Schlageter,  
Markus

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

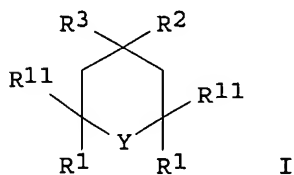
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 775684	A1	19970528	EP 1996-118157	19961113
EP 775684	B1	19990818		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
US 5821374	A	19981013	US 1996-747944	19961112
CN 1156713	A	19970813	CN 1996-114464	19961113
CN 1073074	B	20011017		
AT 183492	E	19990915	AT 1996-118157	19961113
ES 2136930	T3	19991201	ES 1996-118157	19961113
JP 09169685	A2	19970630	JP 1996-304291	19961115
			CH 1995-3291	19951121

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 127:65794

GI



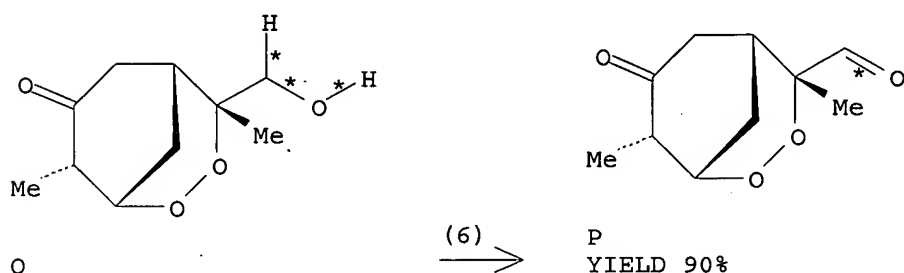
AB Primary and secondary alcs. are oxidized using organic N-chloro compds. in the presence of cyclic amine derivs (I; R<sub>1</sub>, R<sub>11</sub> = alkyl; R<sub>2</sub>, R<sub>3</sub> = H, alkoxy, OH, alkylcarbonyloxy, arylcarbonyloxy, alkylcarbonylamino; R<sub>2</sub>R<sub>3</sub> =

Updated Search

10509228

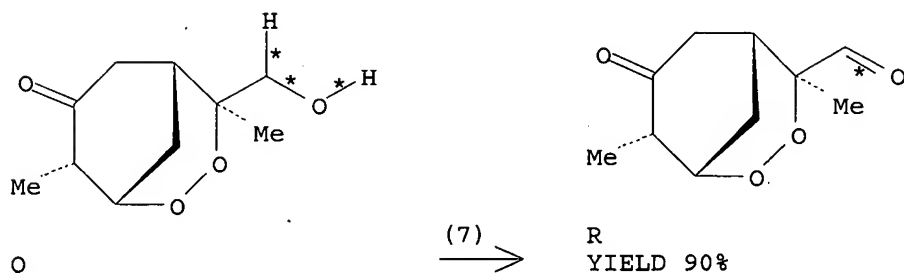
ketal group; Y = N+:O X-, NOH, NO·; X- = anion). Thus, a mixture of (1S,4R,5R,8S)-4-hydroxymethyl-4,8-dimethyl-2,3-dioxabicyclo[3.3.1]nonane-7-one 46.2% and (1S,4S,5R,8S)-4-hydroxymethyl-4,8-dimethyl-2,3-dioxabicyclo[3.3.1]nonane-7-one 47.5% together with NaOAc and trichloroisocyanuric acid in CH<sub>2</sub>Cl<sub>2</sub> at 0° was treated with TEMPO in CH<sub>2</sub>Cl<sub>2</sub> and the mixture was stirred 5 h at 0-3° to give >90% crude yield of (1S,4R,5R,8S)-4,8-dimethyl-7-oxo-2,3-dioxabicyclo[3.3.1]nonane-4-carboxaldehyde 42.3% and (1S,4S,5R,8S)-4,8-dimethyl-7-oxo-2,3-dioxabicyclo[3.3.1]nonane-4-carboxaldehyde 45.8%.

RX(6) OF 7 O ==> P



RX(6) RCT O 160420-93-9  
RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2  
Me4-piperidoxyl, E 127-09-3 AcONa  
PRO P 160497-32-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(7) OF 7 Q ==> R



RX(7) RCT Q 191406-57-2  
RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2  
Me4-piperidoxyl, E 127-09-3 AcONa  
PRO R 160497-33-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

L3 ANSWER 33 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 123:9432 CASREACT  
TITLE: Method of preparing enantiomerically pure

Updated Search

10509228

INVENTOR(S): 3-methyl-5-[1-alkyl-2(S)-pyrrolidinyl]isoxazoles  
 Lin, Nan-Horng; He, Yun; Elliott, Richard L.;  
 Chorghade, Mukund S.; Wittenberger, Steven J.;  
 Bunnelle, William H.; Narayanan, Bikshandar A.;  
 Singam, Pulla R.; Esch, Thomas K. J.; et al.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 41 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

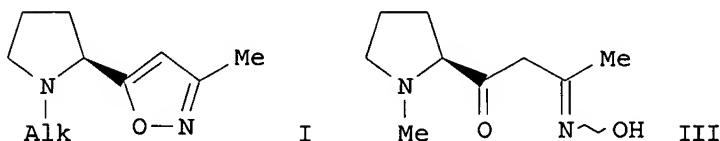
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9507277	A1	19950316	WO 1994-US9734	19940830
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5424444	A	19950613	US 1994-234442	19940428
EP 717741	A1	19960626	EP 1994-931741	19940830
EP 717741	B1	20010530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09502439	T2	19970311	JP 1994-508711	19940830
GR 3036387	T3	20011130	GR 2001-401243	20010814
PRIORITY APPLN. INFO.:			US 1993-117819	19930908
			US 1994-234442	19940428
			US 1992-981587	19921125
			WO 1994-US9734	19940830

OTHER SOURCE(S): MARPAT 123:9432

GI



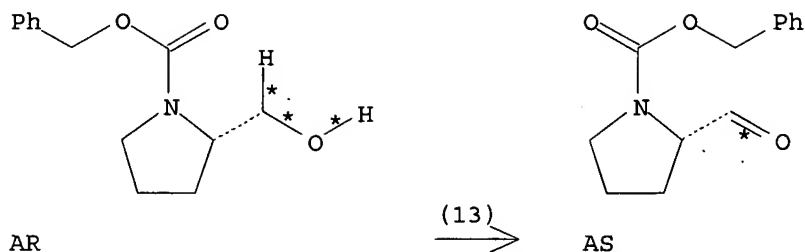
AB Several novel processes for preparing enantiomerically pure title compds. I [Alk = C1-3 alkyl] in high yield are described. I are known cholinergic ligands with selectivity for neuronal nicotinic receptors (no data). In the new methods, a protected pyrrolidine or 2-oxopyrrolidine starting material reacts with a suitable organic anion, and a resulting  $\beta$ -keto oxime intermediate is cyclized and dehydrated. For example, L-proline reacted with  $\text{SO}_2\text{Cl}_2$  in MeOH, followed by  $\text{HC}(\text{OMe})_3$ , to give the Me ester hydrochloride, which was reductively methylated with aqueous  $\text{H}_2\text{CO}$  and  $\text{H}_2$  over Pd/C to give N-methylproline Me ester (II). Acetone oxime was converted by BuLi in THF to its dianion, which reacted with II to give dione oxime III. Cyclization of III by mesyl chloride and  $\text{Et}_3\text{N}$  in  $\text{CH}_2\text{Cl}_2$  gave I [Alk = Me]. Addnl. preps. are described, on small, intermediate, and large (15 kg) scale.

RX(13) OF 84 ...AR ==> AS...

Updated Search



10509228



RX(13) RCT AR 6216-63-3

STAGE(1)

RGT AT 7647-15-6 NaBr

SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)

RGT AU 2564-83-2 Me<sub>4</sub>-piperidoxyl

STAGE(3)

RGT G 497-19-8 Na<sub>2</sub>CO<sub>3</sub>, AV 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO AS 71461-30-8

L3 ANSWER 34 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 116:20658 CASREACT

TITLE: A general synthetic method for the oxidation of primary alcohols to aldehydes: (S)-(+)-2-methylbutanal

AUTHOR(S): Anelli, Pier Lucio; Montanari, Fernando; Quici, Silvio

CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milan, I-20133, Italy

SOURCE: Organic Syntheses (1990), 69, 212-19

CODEN: ORSYAT; ISSN: 0078-6209

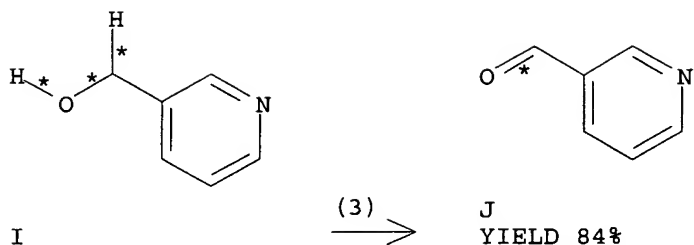
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rapid, inexpensive, selective oxidation of alcs. to aldehydes was achieved by the oxidation of alcs. with sodium hypochlorite in the presence of 2,2,6,6-tetramethylpiperidin-1-oxyl and KBr. The oxidation of (S)-2-methyl-1-butanol with sodium hypochlorite in the presence of 2,2,6,6-tetramethylpiperidin-1-oxyl and KBr gave 82-84% (S)-2-methylbutanal.

RX(3) OF 4 I ==> J

10509228



RX(3) RCT I 100-55-0  
RGT C 7681-52-9 NaOCl, D 2564-83-2 Me4-piperidoxyl, E  
7758-02-3 KBr  
PRO J 500-22-1  
SOL 75-09-2 CH2Cl2

L3 ANSWER 35 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 115:231347 CASREACT

TITLE: Organic oxoammonium salts. 3. A new convenient method for the oxidation of alcohols to aldehydes and ketones

AUTHOR(S): Ma, Zhenkun; Bobbitt, James M.

CORPORATE SOURCE: Dep. Chem., Univ. Connecticut, Storrs, CT, 06269-3060, USA

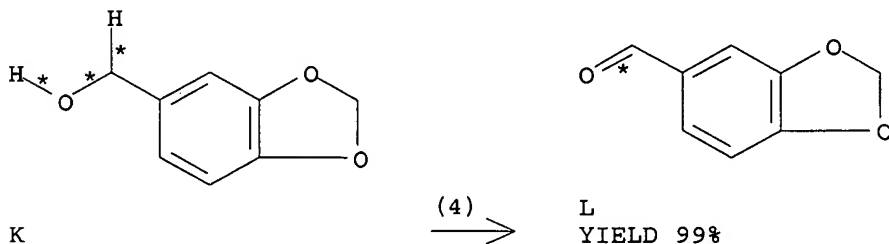
SOURCE: Journal of Organic Chemistry (1991), 56(21), 6110-14  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new method for the selective oxidation of alcs. using organic oxo ammonium salts generated by acid-promoted disproportionation of nitroxides (e.g., 4-acetylamino-2,2,6,6-tetramethylpiperidiny-1-oxyl) in solution were developed. Major advantages are high yields, ease of product isolation, and a high degree of selectivity in the presence of other functional groups.

RX(4) OF 4 K ==> L

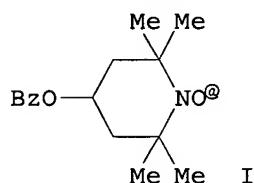


RX(4) RCT K 495-76-1  
RGT C 14691-89-5 1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-, D 104-15-4 TsOH  
PRO L 120-57-0  
SOL 75-09-2 CH2Cl2

Updated Search

10509228

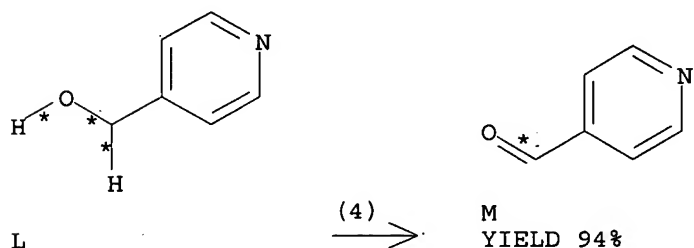
L3 ANSWER 36 OF 38 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 115:113733 CASREACT  
TITLE: A new oxidizing system for aromatic alcohols by the  
combination of N-oxoammonium salt and  
electrosynthesized tetraalkylammonium tribromide  
AUTHOR(S): Inokuchi, Tsutomu; Matsumoto, Sigeaki; Fukushima,  
Mitsuhiro; Torii, Sigeru  
CORPORATE SOURCE: Fac. Eng., Okayama Univ., Okayama, 700, Japan  
SOURCE: Bulletin of the Chemical Society of Japan (1991),  
64(3), 796-800  
CODEN: BCSJA8; ISSN: 0009-2673  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB A combination of piperidinyloxyl I and tetraalkylammonium tribromides (R<sub>4</sub>NBr<sub>3</sub>), which are available from the corresponding tetraalkylammonium bromides via electrooxidn. with KBr, is useful for oxidation of primary and secondary alcs. to aldehydes and ketones, resp. The oxidation proceeds smoothly even with 0.5-1.0 mol % I and 1.5-2.0 equiv of tetraalkylammonium tribromide in an aqueous-organic two-phase solution buffered at pH 8.0-8.6.

This recyclable oxidant/cooxidant system may involve formation of N-oxoammonium salts, the actual oxidizing agents of alcs., by the action of hypobromite species generated from R<sub>4</sub>NBr<sub>3</sub> in the binary solution. Benzylic alcs. bearing electron-releasing groups on the aromatic nucleus are oxidized to aldehydes or ketones without any bromination and overoxidn.

RX(4) OF 4 L ==> M



RX(4) RCT L 586-95-8  
RGT C 3225-26-1 Piperidinoxy deriv., D 38932-80-8  
Bu<sub>4</sub>N.Br<sub>3</sub>, E 127-09-3 AcONa  
PRO M 872-85-5

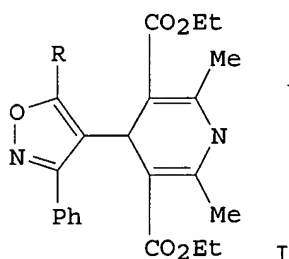
Updated Search

10509228

RX(12) RCT AC 123903-23-1  
RGT D 3225-26-1 Piperidinooxy deriv., E 7486-26-2 NaBrO2,  
C 144-55-8 NaHCO3  
PRO AD 123903-24-2  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

L3 ANSWER 38 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 108:55850 CASREACT  
TITLE: Cardioactivity and solid-state structure of two  
4-isoxazolyldihydropyridines related to the  
4-aryldihydropyridine calcium-channel blockers  
AUTHOR(S): McKenna, John I.; Schlicksupp, Ludwig; Natale,  
Nicholas R.; Willett, Roger D.; Maryanoff, Bruce E.;  
Flaim, Stephen F.  
CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, 83843, USA  
SOURCE: Journal of Medicinal Chemistry (1988), 31(2), 473-6  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

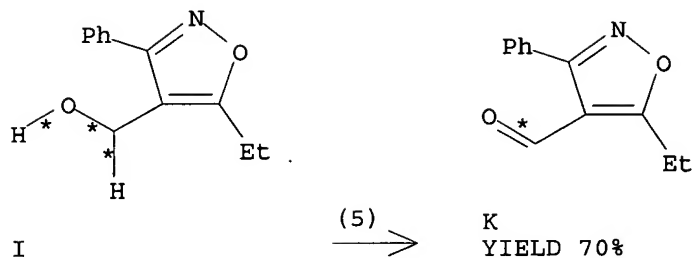


AB Di-Et 2,6-dimethyl-4-(5-ethyl-3-phenyl-4-isoxazolyl)-1,4-dihydropyridine-3,5-dicarboxylate (I, R = Et) and di-Et 2,6-dimethyl-4-(5-isopropyl-3-phenyl-4-isoxazolyl)-1,4-dihydropyridine-3,5-dicarboxylate (I, R = Me2CH) were prepared by Hantzsch cyclization of the isoxazolyl aldehydes with EtO2CCH2Ac and NH3. The mol. structures of I were determined by x-ray crystallog. In I (R = Et), which has an Et group at the C5 position of the isoxazole ring, the deviation from planarity in the dihydropyridine (DHP) ring is the smallest of all known DHP derivs. The dihedral angle between the isoxazole ring and the DHP ring, which is approx. 90° in similar biol. active dihydropyridines, is somewhat smaller (82.7° and 85.2°, resp.) in these two compds. In both compds., one of the ester groups is coplanar with the DHP ring while the other one is out of plane by 14.7° (R = Et) and 18.8° (R = Me2CH). Both I were found to be vasodilators in the Langendorff assay. The potency of I (R = Me2CH) on cardiac flow was similar to that of nifedipine; however, that of I (R = Et) was considerably attenuated. Since isoxazolyl analog I (R = Me2CH) lacks the significant neg. inotropic activity associated with nifedipine, it offers promise as an antihypertensive or antianginal agent.

RX(5) OF 24 ...I ==> K...

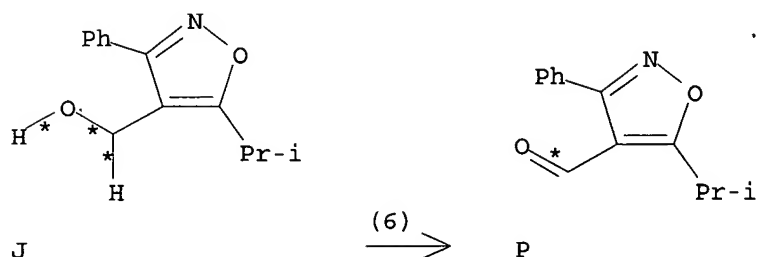
Updated Search

10509228



RX(5) RCT I 99299-07-7  
RGT L 7782-44-7 O2, M 2564-83-2 Me4-piperidoxyl  
PRO K 99298-93-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF

RX(6) OF 24 ...J ==> P...



RX(6) RCT J 99299-09-9  
RGT L 7782-44-7 O2, M 2564-83-2 Me4-piperidoxyl  
PRO P 111525-13-4  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF

=> d his

(FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006)

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 3 S L1  
L3 38 S L1 FULL  
L4 0 S L3 AND SHIOMI, Y?/AU  
L5 0 S L3 AND UNO, O?/AU  
L6 0 S L3 AND OHTA, A?/AU  
L7 0 S L3 AND SUNAKAMI, T?/AU

=> FIL REGISTRY

COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
371.88	372.09

Updated Search

10509228

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-26.98	-26.98

FILE 'REGISTRY' ENTERED AT 19:58:36 ON 12 OCT 2006  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8  
DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 7782-44-7/RN

L8 1 7782-44-7/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L8 SQIDE,1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 7782-44-7 REGISTRY  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Dioxygen  
CN Molecular oxygen  
CN Oxygen molecule  
DR 1338-93-8, 14797-70-7, 80217-98-7, 80937-33-3  
MF O2  
CI COM  
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DDFU, DETHERM\*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA,

Updated Search

10509228

MEDLINE, MRCK\*, MSDS-OHS, PIRA, PROMT, PS, RTECS\*, SPECINFO, TOXCENTER,  
TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VTB

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent;  
Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC  
(Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);  
PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role  
in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical  
study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC  
(Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);  
PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
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MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC  
(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses);  
NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical  
study); BIOL (Biological study); CMBI (Combinatorial study); FORM  
(Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence);  
PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
reagent); USES (Uses)

O—O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

390743 REFERENCES IN FILE CA (1907 TO DATE)

36372 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

391458 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

=> d his

(FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006)

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

L1 STRUCTURE UPLOADED  
L2 3 S L1  
L3 38 S L1 FULL  
L4 0 S L3 AND SHIOMI, Y?/AU  
L5 0 S L3 AND UNO, O?/AU  
L6 0 S L3 AND OHTA, A?/AU  
L7 0 S L3 AND SUNAKAMI, T?/AU

Updated Search

10509228

FILE 'REGISTRY' ENTERED AT 19:58:36 ON 12 OCT 2006  
L8 1 S 7782-44-7/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
3.66	375.75

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-26.98

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FILE CONTENT:1840 - 8 Oct 2006 VOL 145 ISS 15

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\*\*\*\*\*  
\* CASREACT now has more than 10 million reactions \*  
\* \*\*\*\*\*

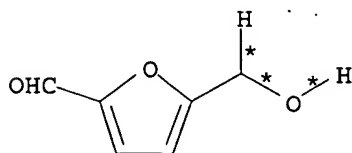
Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

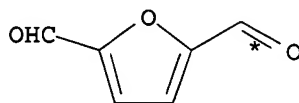
=> d l3, fhit, 1-38

L3 ANSWER 1 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(2) OF 2 A ==> D



A



D  
YIELD 87%

RX(2) RCT A 67-47-0

Updated Search

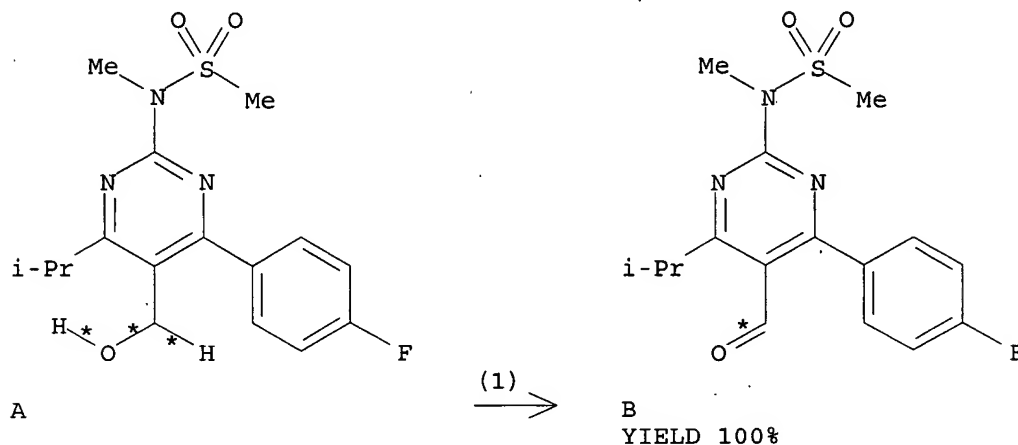


10509228

RGT E 2564-83-2 Me4-piperidoxyl, F 3240-34-4 PhI(OAc)2  
PRO D 823-82-5  
SOL 108-10-1 i-BuCOMe  
CON 1.5 hours, room temperature  
NTE optimization study

L3 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

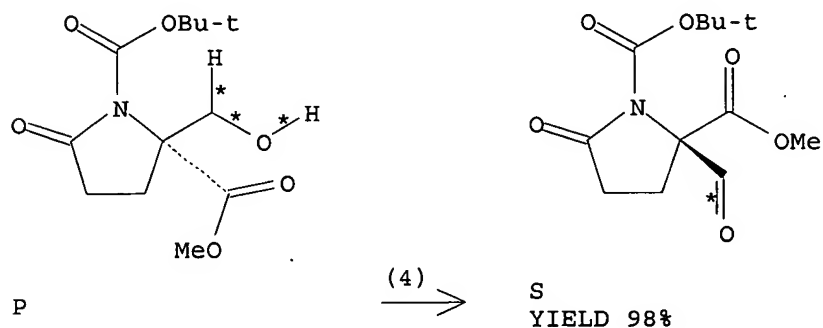
RX(1) OF 11 A ==> B



RX(1) RCT A 147118-36-3  
RGT C 2564-83-2 Me4-piperidoxyl, D 7681-52-9 NaOCl, E 7758-02-3 KBr  
PRO B 147118-37-4  
SOL 7732-18-5 Water, 75-05-8 MeCN  
CON SUBSTAGE(1) 5 deg C  
SUBSTAGE(3) 6 hours  
NTE optimization study

L3 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(4) OF 464 ...P ==> S...



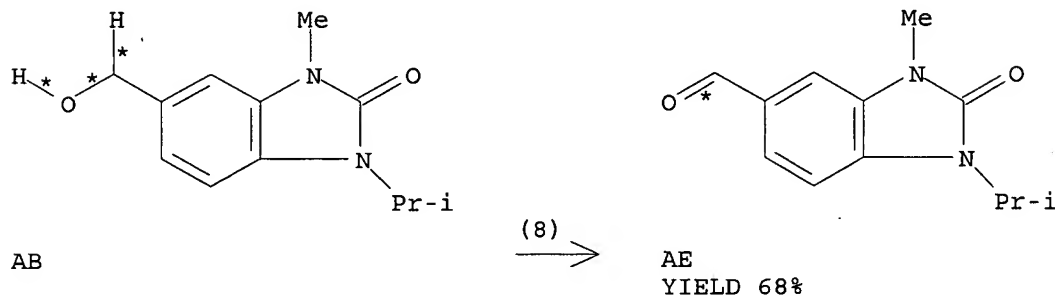
Updated Search

10509228

RX(4) RCT P 866331-68-2  
RGT T 2564-83-2 Me4-piperidoxyl, U 3240-34-4 PhI(OAc)2  
PRO S 866331-49-9  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 26 hours, room temperature

L3 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

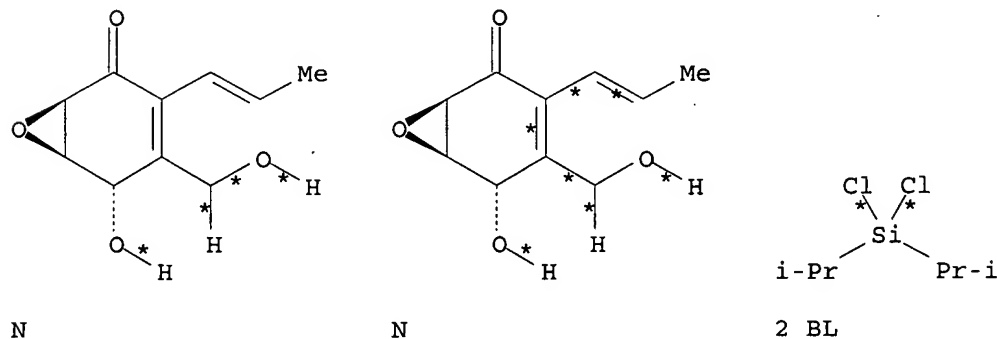
RX(8) OF 71 ...AB ==> AE...



RX(8) RCT AB 865443-84-1  
RGT AF 2564-83-2 Me4-piperidoxyl, AG 128-09-6  
Chlorosuccinimide, AH 1112-67-0 Bu4NCl  
PRO AE 865443-86-3  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 18 hours, 22 deg C, pH 8.6  
NTE buffered solution, sodium bicarbonate-potassium carbonate

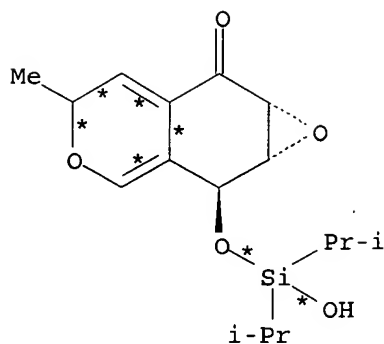
L3 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(25) OF 255 ...2 N + 2 BL ==> BM + BN...

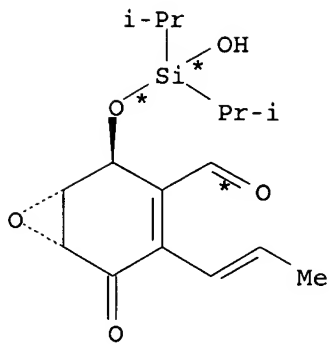


Updated Search

10509228



BM  
YIELD 76%



BN  
YIELD 15%

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me4-piperidoxyl, X 7782-44-7 O2, Y  
7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4  
RGT AY 288-32-4 1H-Imidazole  
SOL 68-12-2 DMF  
CON 15 minutes, 0 deg C

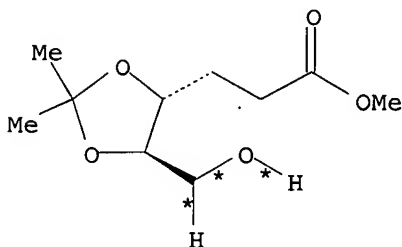
STAGE(3)

RGT L 7732-18-5 Water

PRO BM 668987-33-5, BN 668987-32-4

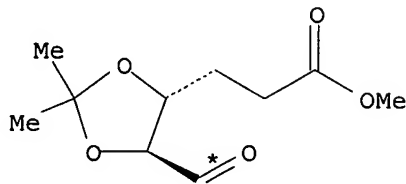
L3 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 171 ...AT ==> AX...



AT

(11)  
→



AX  
YIELD 70%

RX(11) RCT AT 850222-14-9

STAGE(1)

Updated Search

10509228

RGT AY 95407-69-5 1-Piperidinyloxy,  
4-methoxy-2,2,6,6-tetramethyl-, AZ 144-55-8 NaHCO<sub>3</sub>, BA  
7681-52-9 NaOCl, BB 7758-02-3 KBr  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 minutes, 0 deg C

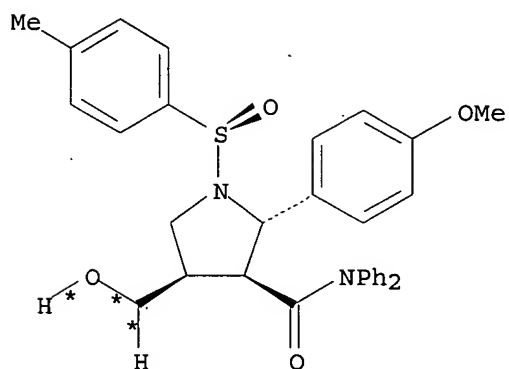
STAGE(2)

RGT O 7772-98-7 Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>  
SOL 7732-18-5 Water

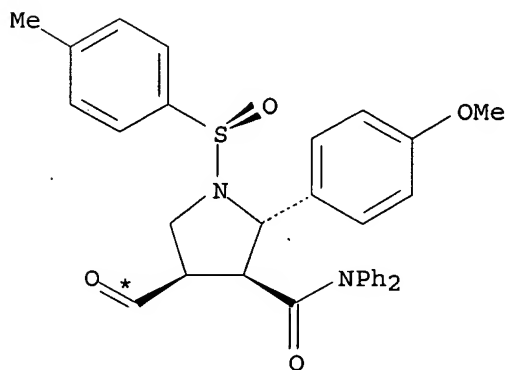
PRO AX 862907-39-9

L3 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 66 ...H ==> L...



H



L

YIELD 91%

RX(3) RCT H 861145-05-3

STAGE(1)

Updated Search

10509228

RGT M 2564-83-2 Me4-piperidoxyl, N 7647-15-6 NaBr  
SOL 7732-18-5 Water, 108-88-3 PhMe, 141-78-6 AcOEt  
CON room temperature -> 0 deg C

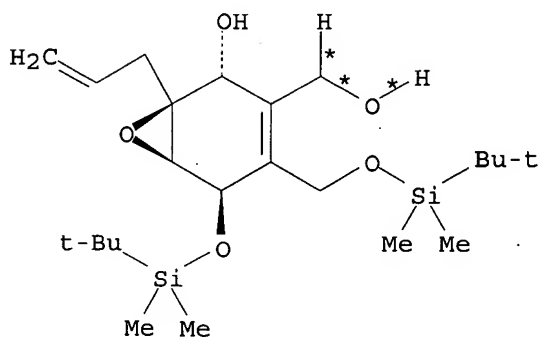
STAGE(2)

RGT O 144-55-8 NaHCO3, P 7681-52-9 NaOCl

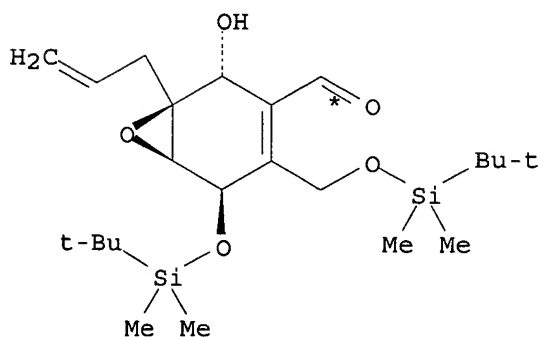
PRO L 861145-06-4

L3 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 105 ...L ==> M...



L



M

YIELD 90%

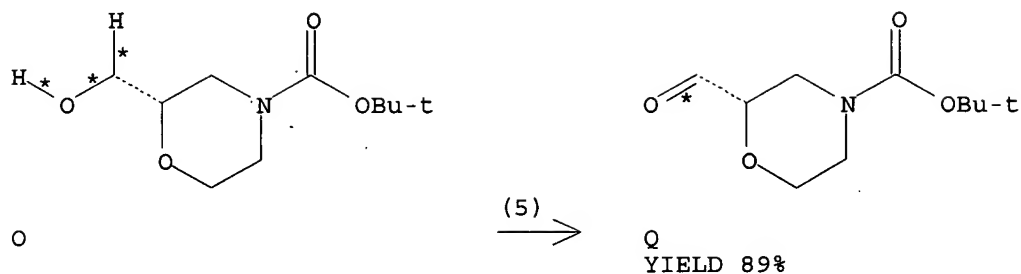
RX(5) RCT L 852392-89-3  
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P  
7758-89-6 CuCl  
PRO M 852392-90-6  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

L3 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

RX(5) OF 81 ...O ==> Q...



RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO<sub>3</sub>

SOL 141-78-6 AcOEt

CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) 1 hour, -5 deg C

SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)<sub>2</sub>

SOL 7732-18-5 Water

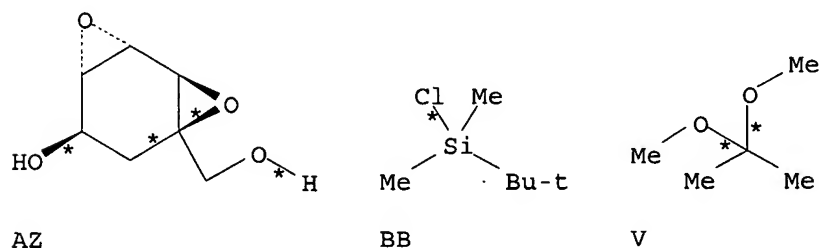
PRO Q 847805-31-6

NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization,  
use of EtOAc suppresses chlorination

L3 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

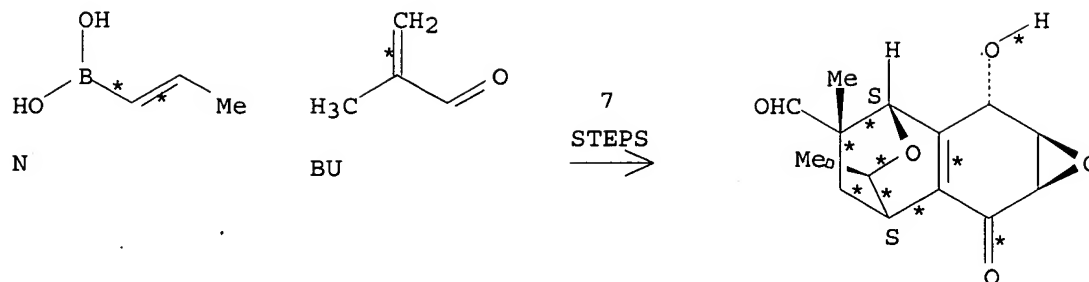
RX(111) OF 236 COMPOSED OF RX(13), RX(5), RX(4), RX(14), RX(3), RX(15), RX(23)

RX(111) AZ + BB + V + N + BU ==> BV



Updated Search

10509228



BV  
YIELD 69%

RX(13) RCT AZ 635678-63-6, BB 18162-48-6  
RGT BC 121-44-8 Et3N, BD 1122-58-3 4-DMAP  
PRO AA 488808-28-2  
SOL 75-09-2 CH2Cl2  
CON 15 hours, room temperature

RX(5) RCT AA 488808-28-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7758-02-3 KBr,  
AD 7681-52-9 NaOCl, AE 144-55-8 NaHCO3  
SOL 75-09-2 CH2Cl2, 7732-18-5 Water  
CON 40 minutes, -10 deg C, pH 9.5

STAGE(2)

RGT AF 7631-86-9 SiO2  
SOL 108-88-3 PhMe  
CON 4.5 hours, 70 deg C

PRO U 488808-29-3

RX(4) RCT U 488808-29-3

STAGE(1)

RGT X 9037-24-5 Amberlyst 15  
SOL 67-56-1 MeOH  
CON 5 hours, room temperature

STAGE(2)

RCT V 77-76-9  
RGT Y 24057-28-1 Pyridinium tosylate  
SOL 75-09-2 CH2Cl2  
CON 4 hours, room temperature

PRO W 488808-30-6

RX(14) RCT W 488808-30-6  
RGT AT 7553-56-2 I2, BE 2712-78-9 PhI(O2CCF3)2, BF 110-86-1 Pyridine  
PRO M 488808-31-7  
SOL 75-09-2 CH2Cl2  
CON 22 hours, room temperature  
NTE in the dark

Updated Search

10509228

RX(3) RCT M 488808-31-7, N 7547-97-9

STAGE(1)

CAT 14220-64-5 PdCl<sub>2</sub>(PhCN)<sub>2</sub>, 20667-12-3 Ag<sub>2</sub>O, 603-32-7 Ph<sub>3</sub>As  
SOL 109-99-9 THF, 7732-18-5 Water  
CON 11 hours, room temperature

STAGE(2)

RGT P 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water  
CON 1 hour, room temperature

PRO O 238424-99-2  
NTE in the dark

RX(15) RCT O 238424-99-2  
RGT X 9037-24-5 Amberlyst 15  
PRO G 238424-94-7  
SOL 67-56-1 MeOH  
CON 40 minutes, room temperature

RX(23) RCT G 238424-94-7

STAGE(1)

RGT K 1313-13-9 MnO<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, 0 deg C

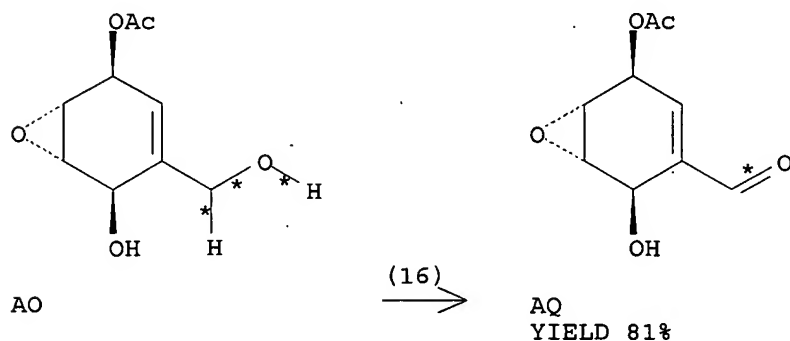
STAGE(2)

RCT BU 78-85-3  
CON room temperature

PRO BV 832731-77-8  
NTE stereoselective

L3 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(16) OF 185 ...AO ==> AQ...



RX(16) RCT AO 792910-40-8  
RGT AR 2564-83-2 Me<sub>4</sub>-piperidoxyl, AS 7758-89-6 CuCl, AT  
7782-44-7 O<sub>2</sub>  
PRO AQ 792910-42-0

Updated Search

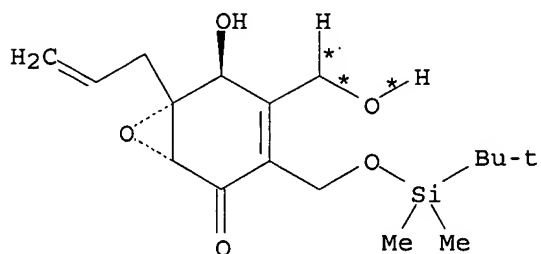


10509228

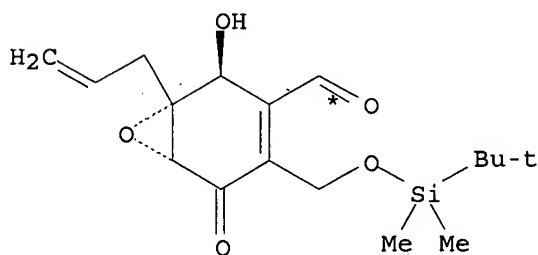
SOL 68-12-2 DMF  
CON room temperature

L3 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(9) OF 230 ...Y ==> AA...



Y



AA  
YIELD 90%

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4  
SOL 7732-18-5 Water

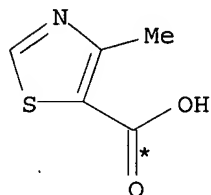
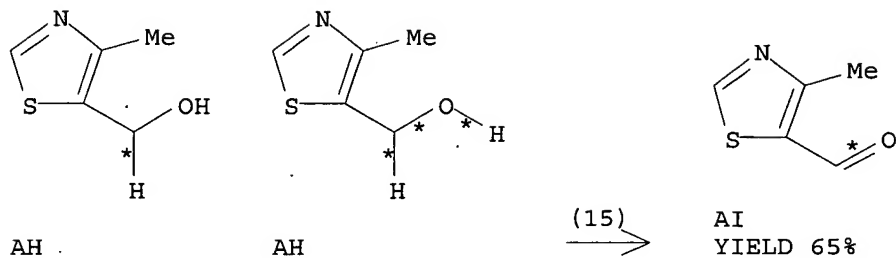
PRO AA 791854-32-5  
NTE chemoselective

L3 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(15) OF 33 2 AH ==> AI + AJ

Updated Search

10509228



AJ  
YIELD 11%

RX(15) RCT AH 1977-06-6

STAGE(1)

RGT C 3225-26-1 Piperidinooxy deriv., D 7631-86-9  
SiO2

SOL 67-64-1 Me2CO

CON 10 minutes, room temperature

STAGE(2)

RGT E 7681-52-9 NaOCl

SOL 7732-18-5 Water

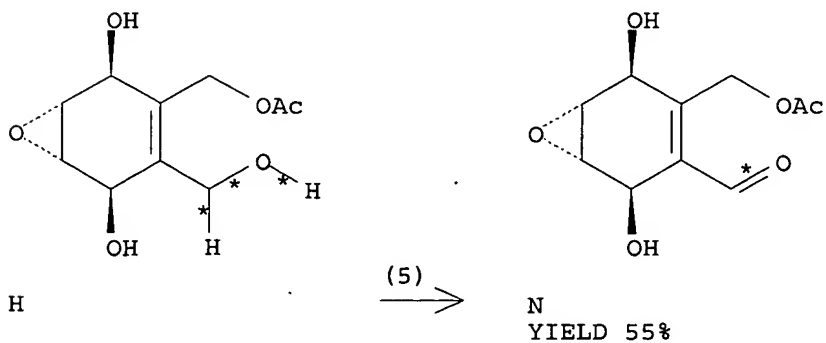
CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 2 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

L3 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 87 ...H ==> N...



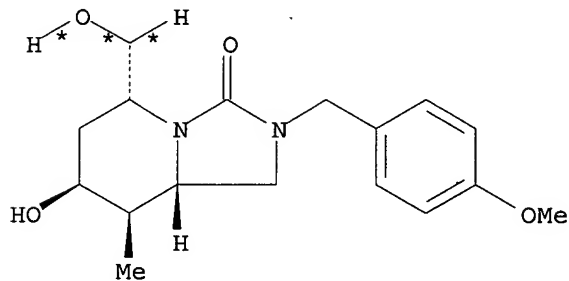
Updated Search

10509228

RX(5) RCT H 735317-25-6  
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q  
7758-89-6 CuCl  
PRO N 735317-27-8  
SOL 68-12-2 DMF

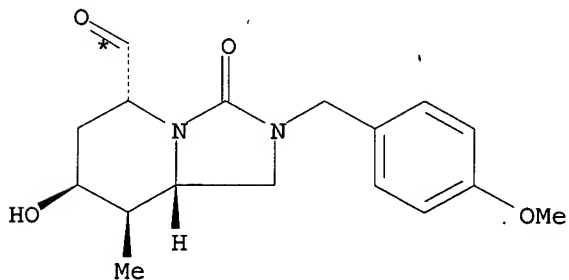
L3 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 120 ...V ==> H...



V

(6) →



H

YIELD 75%

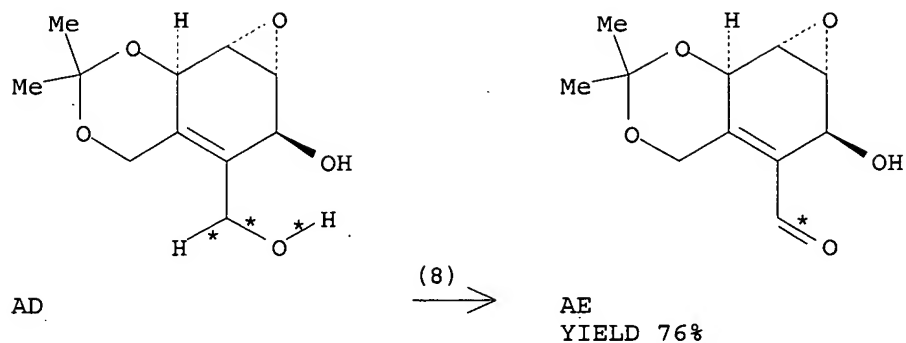
RX(6) RCT V 732278-69-2  
RGT W 3240-34-4 PhI(OAc)2, X 2564-83-2 Me4-piperidoxyl, Y  
75-75-2 MeSO3H  
PRO H 732278-68-1  
SOL 865-49-6 CDCl3  
CON 3 hours, room temperature

L3 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(8) OF 307 ...AD ==> AE...

Updated Search

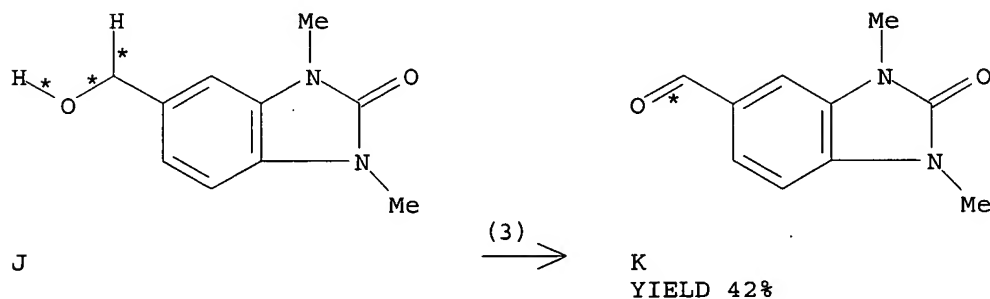
10509228



RX(8) RCT AD 701921-79-1  
RGT AF 7782-44-7 O<sub>2</sub>, AG 7758-89-6 CuCl, AH 2564-83-2  
Me<sub>4</sub>-piperidoxyl  
PRO AE 701921-80-4  
SOL 68-12-2 DMF

L3 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 443 ...J ==> K...

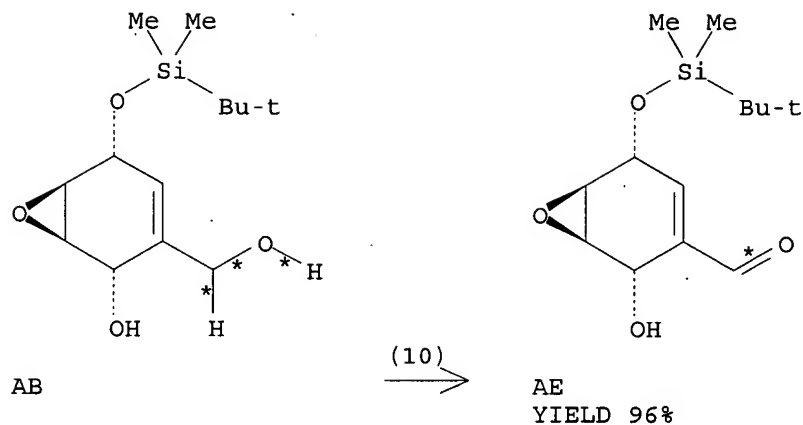


RX(3) RCT J 345657-96-7  
RGT L 2564-83-2 Me<sub>4</sub>-piperidoxyl, M 128-09-6  
Chlorosuccinimide  
PRO K 55241-49-1  
CAT 1112-67-0 Bu<sub>4</sub>NCl  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 5.5 hours, room temperature, pH 8.6  
NTE buffered soln.

L3 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(10) OF 115 ...AB ==> AE...

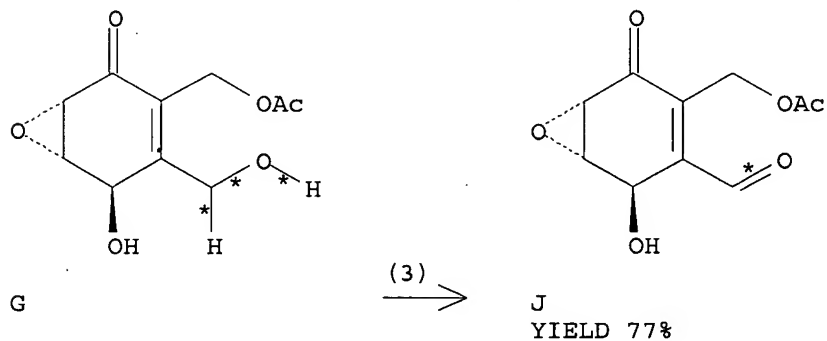
10509228



RX(10) RCT AB 678197-28-9  
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH 7758-89-6 CuCl  
PRO AE 678197-29-0  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

L3 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 100 ...G ==> J...



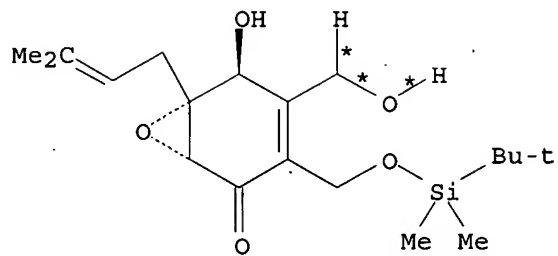
RX(3) RCT G 676263-76-6  
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2  
PRO J 676263-78-8  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON room temperature  
NTE chemoselective

L3 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 201 ...AF ==> AH...

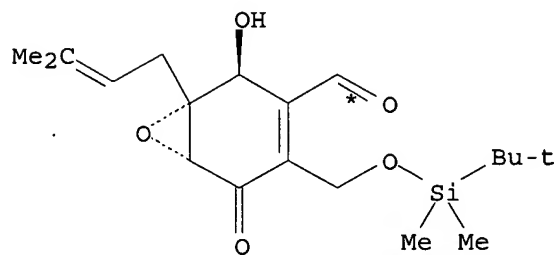
Updated Search

10509228



AF

(11)  $\longrightarrow$



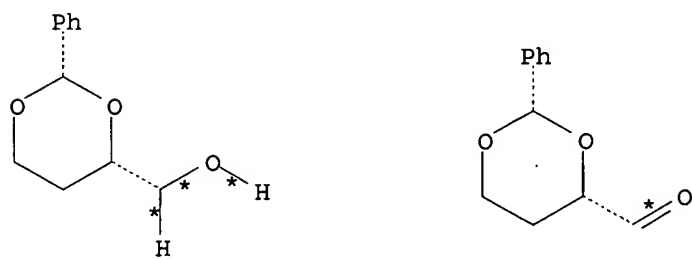
AH

YIELD 90%

RX(11) RCT AF 674358-50-0  
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2  
PRO AH 674358-53-3  
CAT 7758-89-6 CuCl  
SOL 68-12-2 DMF  
CON 3 hours, room temperature  
NTE chemoselective

L3 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 288 ...M ==> N...



M

(3)  $\longrightarrow$

N  
YIELD 70%

RX(3) RCT M 103773-79-1

Updated Search

10509228

STAGE(1)

RGT O 3240-34-4  $\text{PhI}(\text{OAc})_2$ , P 14691-89-5  
1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-  
SOL 75-09-2  $\text{CH}_2\text{Cl}_2$   
CON 14 hours, 18 deg C

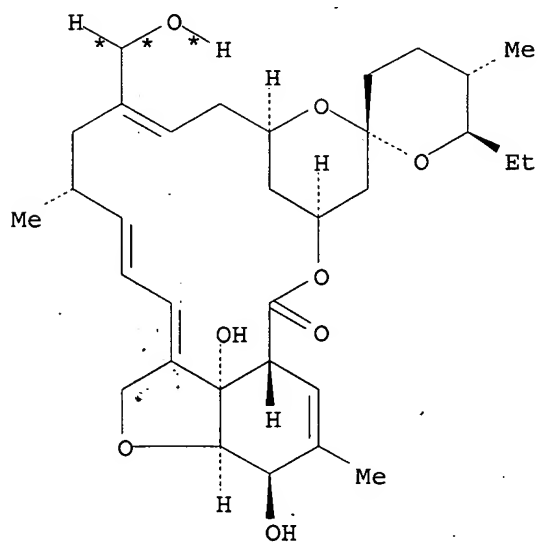
STAGE(2)

RGT E 144-55-8  $\text{NaHCO}_3$   
SOL 7732-18-5 Water  
CON 18 deg C

PRO N 145958-02-7

L3 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 28 ...K ==> M...

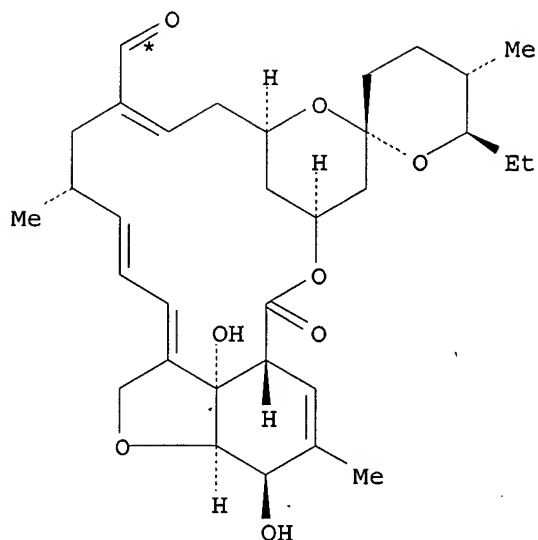


K

(5)  $\longrightarrow$

Updated Search

10509228

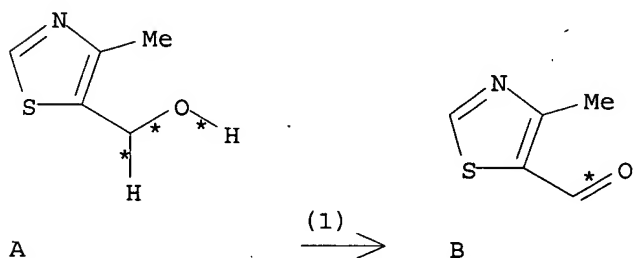


M  
YIELD 87%

RX(5) RCT K 112774-81-9  
RGT N 144-55-8 NaHCO<sub>3</sub>, O 584-08-7 K<sub>2</sub>CO<sub>3</sub>, P 2564-83-2  
Me<sub>4</sub>-piperidoxyl, Q 1112-67-0 Bu<sub>4</sub>NCl, R 128-09-6  
Chlorosuccinimide  
PRO M 112774-92-2  
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature  
NTE regioselective

L3 ANSWER 23 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 5 ...A ==> B



RX(1) RCT A 1977-06-6  
STAGE(1)  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 5 minutes, room temperature  
STAGE(2)  
RGT C 144-55-8 NaHCO<sub>3</sub>

Updated Search



10509228

SOL 7732-18-5 Water  
CON SUBSTAGE(1) 30 - 32 deg C  
SUBSTAGE(2) 5 - 10 minutes, 30 - 32 deg C

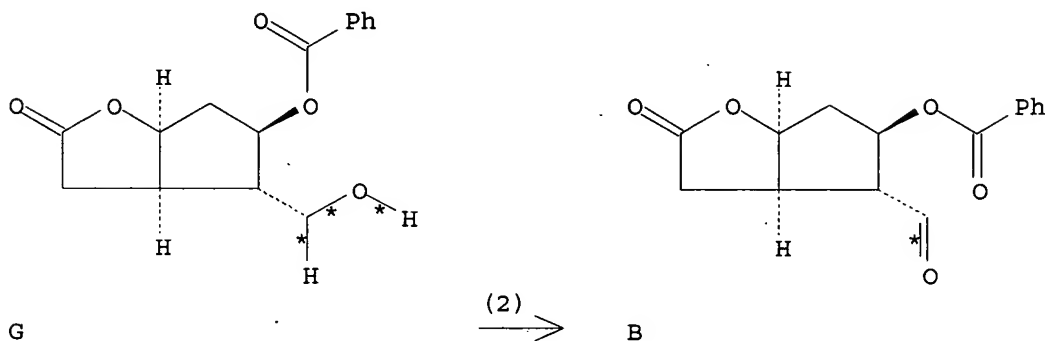
STAGE(3)

RGT D 7758-02-3 KBr, E 2564-83-2 Me4-piperidoxyl, F  
7681-52-9 NaOCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 32 deg C -> 0 deg C  
SUBSTAGE(3) 1 hour, 0 - 2 deg C  
SUBSTAGE(4) 0 - 2 deg C

PRO B 82294-70-0

L3 ANSWER 24 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

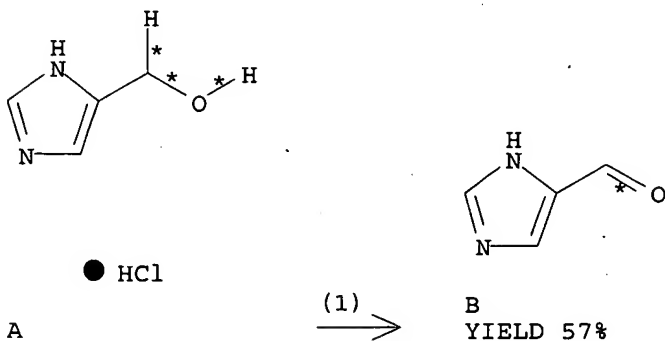
RX(2) OF 66 G ==> B...



RX(2) RCT G 39746-00-4  
RGT H 7681-52-9 NaOCl, I 2564-83-2 Me4-piperidoxyl, J  
7758-02-3 KBr  
PRO B 39746-01-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

L3 ANSWER 25 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 3 A ==> B



Updated Search

10509228

RX(1) RCT A 32673-41-9

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,  
4-hydroxy-2,2,6,6-tetramethyl-  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

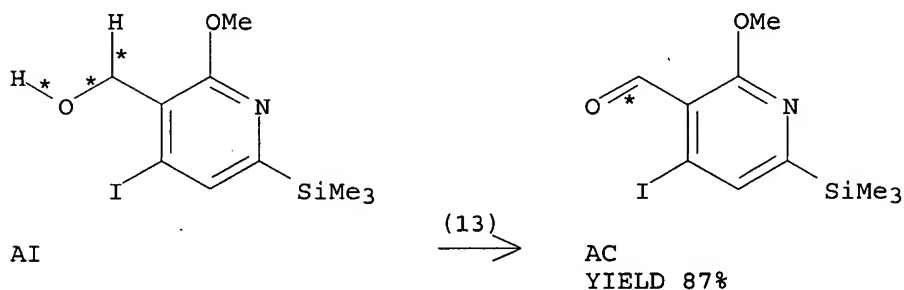
STAGE(2)

RGT D 7681-52-9 NaOCl  
SOL 7732-18-5 Water

PRO B 3034-50-2

L3 ANSWER 26 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(13) OF 249 AI ==> AC

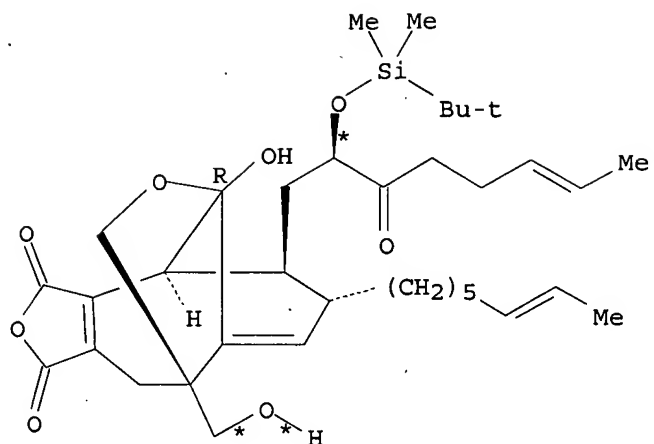


RX(13) RCT AI 375346-05-7  
RGT AO 7681-52-9 NaOCl, AP 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AC 174092-75-2  
SOL 7732-18-5 Water, 108-88-3 PhMe  
NTE oxidn. at 0-5° for 2 h

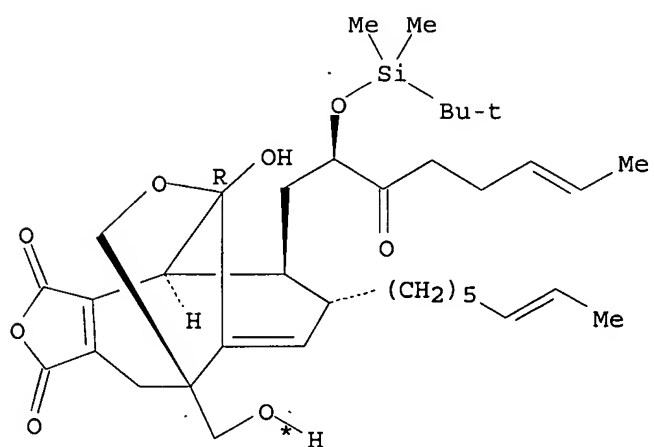
L3 ANSWER 27 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(362) OF 443 COMPOSED OF RX(38), RX(39), RX(40), RX(1), RX(43)  
RX(362) 2 I + 2 BX + BA ==> DI

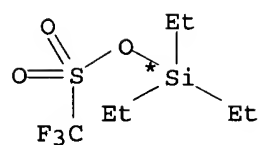
10509228



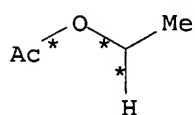
I



I



2 BX

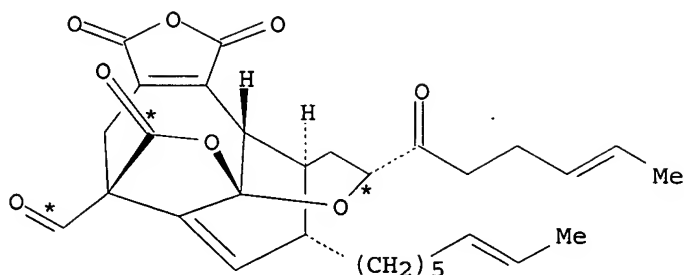


BA

5  
STEPS  
→

Updated Search

10509228



DI  
YIELD 95%

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent  
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6  
RGT P 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me<sub>4</sub>-piperidoxyl, DE 3240-34-4  
PhI(OAc)<sub>2</sub>  
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 7732-18-5 Water

Updated Search

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STAGE(2)

RGT D 75-75-2 MeSO<sub>3</sub>H

SOL 67-66-3 CHCl<sub>3</sub>

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

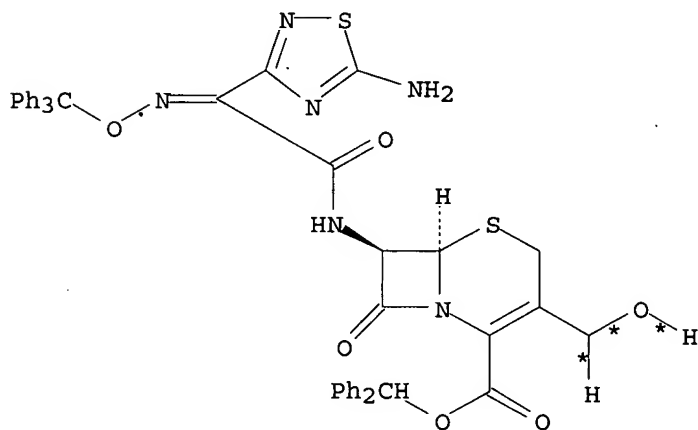
STAGE(2)

RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

L3 ANSWER 28 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

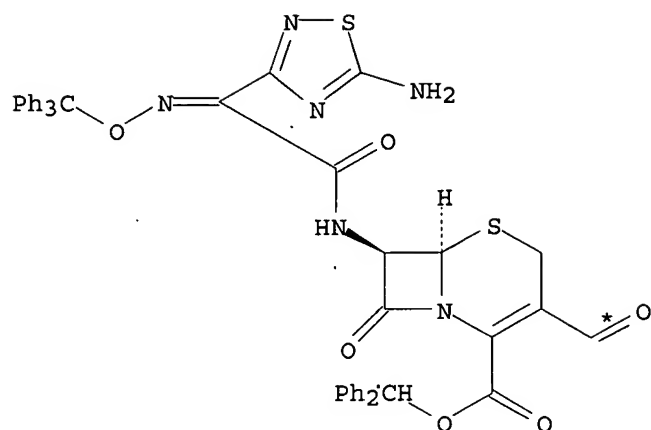
RX(2) OF 29 ...D ==> G...



D

(2) →

10509228



G

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO3, J 2564-83-2

Me4-piperidoxyl

SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT K 7681-52-9 NaOCl

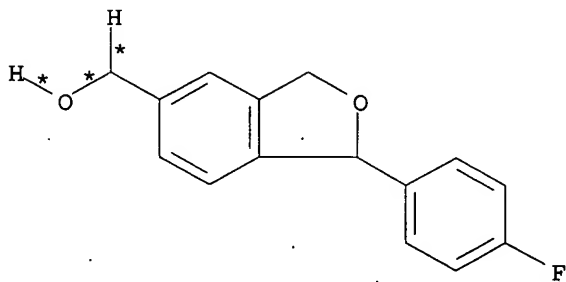
SOL 7732-18-5 Water

PRO G 376653-37-1

NTE alternative prepn. shown

L3 ANSWER 29 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 28 ...U ==> Z...

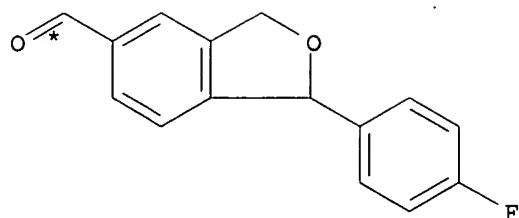


U

(6) >

Updated Search

10509228



Z  
YIELD 84%

RX(6) RCT U 335612-71-0

STAGE(1)

RGT AA 144-55-8 NaHCO<sub>3</sub>, AB 1643-19-2 Bu<sub>4</sub>N.Br, AC  
2564-83-2 Me<sub>4</sub>-piperidoxyl  
SOL 141-78-6 AcOEt

STAGE(2)

RGT AD 7681-52-9 NaOCl  
SOL 7732-18-5 Water

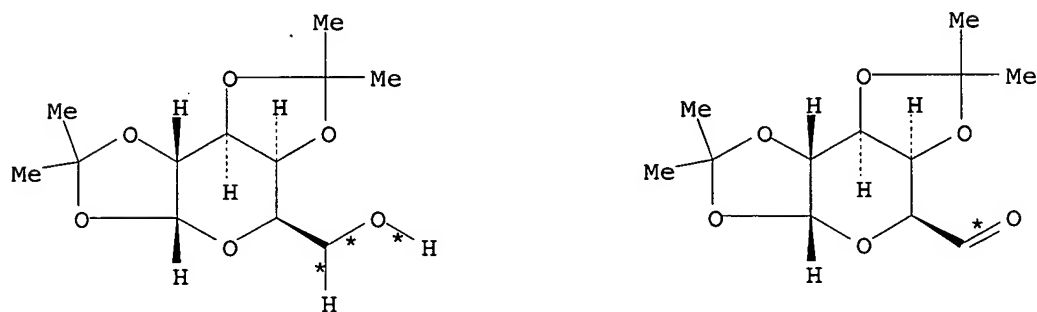
STAGE(3)

SOL 7732-18-5 Water

PRO. Z 335612-72-1

L3 ANSWER 30 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 18 AC ==> AD



AC

(11)

AD  
YIELD 97%

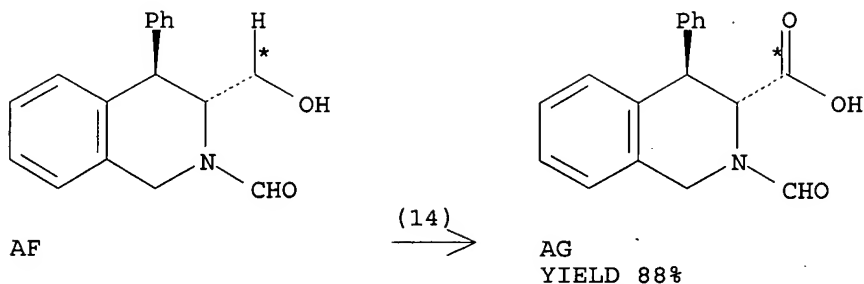
RX(11) RCT AC 4064-06-6  
RGT D 74-89-5D MeNH<sub>2</sub>, J 2564-83-2 Me<sub>4</sub>-piperidoxyl  
PRO AD 4933-77-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE STEREOSELECTIVE

L3 ANSWER 31 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

RX(14) OF 52 ...AF ==> AG...



RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO<sub>3</sub>,

AJ 7758-02-3 KBr, AK 1112-67-0 Bu<sub>4</sub>NCl

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO<sub>3</sub>, AM 7647-14-5 NaCl

SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

STAGE(5)

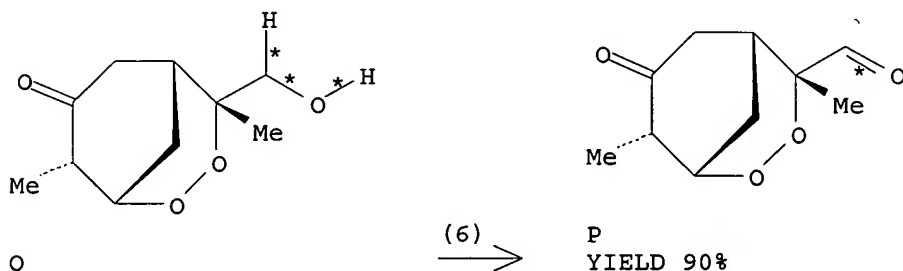
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

PRO AG 294869-51-5

NTE STEREOSELECTIVE

L3 ANSWER 32 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 7 O ==> P



RX(6) RCT O 160420-93-9

RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2

Updated Search

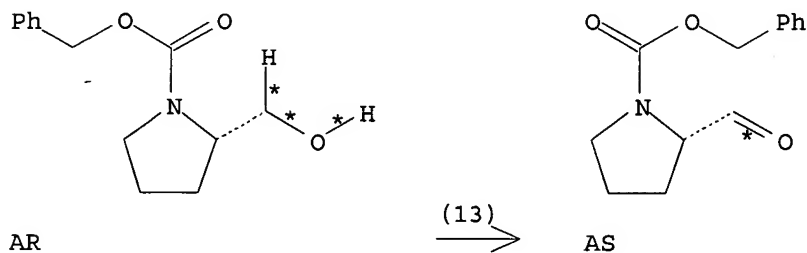


10509228

Me4-piperidoxyl, E 127-09-3 AcONa  
PRO P 160497-32-5  
SOL 75-09-2 CH2Cl2

L3 ANSWER 33 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(13) OF 84 ...AR ==> AS...



RX(13) RCT AR 6216-63-3

STAGE(1)

RGT AT 7647-15-6 NaBr

SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)

RGT AU 2564-83-2 Me4-piperidoxyl

STAGE(3)

RGT G 497-19-8 Na2CO3, AV 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO AS 71461-30-8

L3 ANSWER 34 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 4 I ==> J

<-----User Break----->

=> d his

(FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006)

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 38 S L1 FULL

L4 0 S L3 AND SHIOMI, Y?/AU

L5 0 S L3 AND UNO, O?/AU

L6 0 S L3 AND OHTA, A?/AU

L7 0 S L3 AND SUNAKAMI, T?/AU

FILE 'REGISTRY' ENTERED AT 19:58:36 ON 12 OCT 2006

L8 1 S 7782-44-7/RN

SET NOTICE 1 DISPLAY

Updated Search

10509228

SET NOTICE LOGIN DISPLAY

FILE 'CASREACT' ENTERED AT 20:01:06 ON 12 OCT 2006

=> d l3, ibib abs fhlt, 1-38

COMMAND INTERRUPTED

REENTER FILE 'CASREACT'

AND TRY AGAIN, OR ENTER '?' FOR MORE INFORMATION.

Your command did not complete due to a temporary system problem. To recover, reenter the file you are in now. Then, any command that is normally available to you may be used. No cost summary for the current file will be displayed. After reentering the current file you may retry your command. Also, you may wish to SAVE your search query. This can be done in any file. If you cannot access your current file, or if your command fails a second time, notify the Help Desk. Enter "HELP STN" for information on contacting the nearest STN Help Desk by telephone or by using the SEND command in STNMAIL file.

=> d l3, ibib fhlt, all

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> d l3, ibib abs fhlt

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands

## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	919	((549/70) or (546/315)).CCLS.	US-PGPUB; USPAT	OR	OFF	2006/10/12 22:28
L2	92	1 and heterocyclic and aldehyde	USPAT	OR	OFF	2006/10/12 22:30
L3	123	1 and heterocyclic and aldehyde	US-PGPUB; USPAT	OR	OFF	2006/10/12 22:30